

Department of Chemical Engineering

**Modelling and Control Strategies for Extractive Alcoholic
Fermentation: Partial Control Approach**

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**This thesis is presented for the Degree of
Doctor of Philosophy of Curtin University**

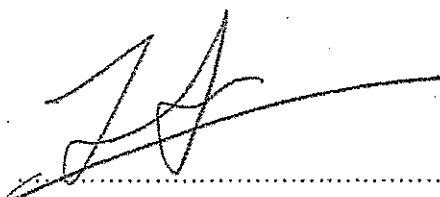
November 2010

Declaration

To the best of my knowledge and belief this thesis contains no material previously published by any other person except where due acknowledgment has been made.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any university.

Signature:

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Date:

25 / 11 / 2010

And yet, I am quite ready to admit that there is a method which might be described as “the one method of philosophy”. But it is not characteristic of philosophy alone; it is, rather, the one method of all rational discussion, and therefore of the natural sciences as well as of philosophy. The method I have in mind is that of stating one’s problem clearly and of examining its various proposed solution critically.

Karl Popper

The Logic of Scientific Discovery

Abstract

The vast majority of chemical and bio-chemical process plants are normally characterized by large number of measurements and relatively small number of manipulated variables; these *thin* plants have more output than input variables. As the number of manipulated variables restricts the number of controlled variables, thin plant has presented a daunting challenge to the engineers in selecting which measured variables to be controlled. In general, this is an important problem in modern process control today, because controlled variables selection is one of the key questions which must be carefully addressed in order to effectively design control strategies for process plants. While the issue relating to controlled variables selection has remained the key question to be resolved since the articulation of CSD problem by Foss in 1970s, the work described in this thesis points out to another equally important question in CSD, that is, what is the *sufficient number* of controlled variables required? Thinking over this question leads one to the necessity for gaining a rational understating of the *governing principle* in partial control design, namely the *variables interaction*.

In this thesis, we propose a novel *data-oriented* approach to solving the control structure problem within the context of partial control framework. This approach represents a significant departure from the mainstream methods in CSD, which currently can be broadly classified into two major categories as the *mathematical-oriented* and *heuristic-hierarchical* approaches. The key distinguishing feature of the proposed approach lies in its adoption of technique based on the Principal Component Analysis (PCA), which is used to systematically determine the suitable controlled variables. Conversely, the determination of the controlled variables in mathematical-oriented and heuristic-hierarchical approaches is done via the mathematical optimization and process knowledge/engineering experience, respectively. It is important to note that, the data-oriented approach in this thesis emerges from the fusion of two important concepts, namely the partial control structure and PCA. While partial control concept provides the sound theoretical framework for addressing the CSD problem in a systematic manner,

the PCA-based technique helps in determining not only the suitable controlled variables but also the sufficient number of controlled variables required.

Since the classical framework of partial control is not amendable to a systematic way in the identification of controlled variables, it is necessary to develop a new framework of partial control in this thesis. Within this new framework the *dominant variable* can be clearly defined, and which in turn allows the incorporation of PCA-based technique for the systematic identification of controlled variables.

The application of the data-oriented approach is demonstrated on a nonlinear multivariable bioprocess case study, called the two-stage continuous extractive (TSCE) alcoholic fermentation process. The system consists of 5 interlinked units: 2 bioreactors in series, a centrifuge, vacuum flash vessel and treatment tank. The comparison of the two-stage design with that of single-stage design reported in literature shows that: (1) both designs exhibit comparable performance in term of the maximum allowable *trade-off* values between yield and productivity, and (2) two-stage design exhibits stronger nonlinear behaviour than that of single-stage. Thus, the design of control strategies for the former is expected to be more challenging.

Various partial control strategies are developed for the case study, such as basic partial control strategy, complete partial control strategies with and without PID enhancement technique and optimal size partial control strategy. Note that, this system consists of 16 output variables and only 6 potential manipulated variables, which has approximately 4,000,000 control structure alternatives. Therefore, the application of mathematical approach relying on optimization is not practical for this case study – i.e. assuming that evaluation of each alternative takes 30 seconds of optimization time, thus, complete screening will require almost 4 years to complete.

Several exciting new insights crystallize from the simulation study performed on the case study, where two of them are most important from the perspective of effective design of partial control strategy:

- 1) There is an optimal size of partial control structure where too many controlled variables can lead to the presence of *bottleneck control-loop*, which in turn can severely limit the dynamic response of overall control system. On the other

hand, too few controlled variables can lead to unacceptable variation or loss in performance measures.

- 2) The nature of variables interaction depends on the choice of control structure. Thus, it is important to ensure that the nature of open-loop variables interaction is preserved by the implementation of a particular control strategy. When this is achieved, then we say that this control system works *synergistically* with the *inherent* control capability of a given process – i.e. achieving the *synergistic external-inherent control system* condition.

The proposed approach has been successfully applied to the case study, where the optimal partial control structure is found to be 3x3 i.e. 3 controlled variables are sufficient to meet all 3 types of control objectives: overall (implicit) performance objectives, constraint and inventory control objectives. Finally, the proposed approach effectively unifies the advantages of both mathematical-oriented and heuristic-hierarchical approaches, and while at the same time capable of overcoming many limitations faced by these two mainstream approaches.

Acknowledgments

I wish to thank my supervisors, Professor Yudi Samyudia and Professor Moses O. Tadé, for their continuous support and guidance throughout my research study. I am really grateful to both of them because they have given me the freedom to venture into a research area endowed with problems which are both challenging and exciting. Also I would like to express my appreciation to Associate Professor Chua Han Bing who has given me some valuable advices regarding the fermentation process.

I would like to acknowledge the Malaysian Ministry of Science, Technology and Innovation (MOSTI) for supporting this research study through the eScienceFund project (no: 02-02-07-SF0001). And I am also grateful to Emily who has given me support to complete this project. Moreover, I would like to acknowledge Curtin University, Sarawak Campus for providing the scholarship to pursue this study.

I would like to thank my friends, to those who already exited and who remain, who have made “Lutong Gathering” a happy part of my day for years at Curtin Sarawak – from the days when it was started by Fook Wing Chau, Freddie Panau, Rama, Nabil and Nader, and later joined by Tan Ka Kheng, Osama Twig, Zang Zhuquan and recently by Shamsul Anwar, Aaron and Bejay. Their companionship has been a fountain of moral support that has to a certain extent contributed to the timely completion of this thesis.

Especially, I wish to thank Antonia for her great support, patience and loving care. Finally, most of all, I am indebted to my father and my late mother for the tremendous kindness and love that they have given me. To them I humbly dedicate this thesis.

Author Biography

Jobrun Nandong received his MEng degree in Chemical Engineering from Imperial College in 1999. After graduation he worked at the Ministry of Industrial Development as Technical Project Engineer in charge of the supervision of the industrial estate development in the state of Sarawak. In 2001 he changed to academic position when he moved to Curtin University Sarawak Campus, which is an offshore campus of the Curtin University of Technology, Australia. He decided to pursue a part-time PhD study in 2006 under the supervision of Professor Yudi Samyudia and Professor Moses Tadé in the area of process control. In the same year, he also managed to secure a national grant from the Malaysia Ministry of Science, Technology and Innovation (MOSTI), which provided a financial support for this research study. Currently he is a senior lecturer in the Chemical Engineering Department of Curtin University, Sarawak Campus. His research interests are in the modelling and control of biotechnological processes, biofuels production and wastewater treatment.

Publications arising from this thesis

J. Nandong, Y. Samyudia and M.O. Tadé, Optimal partial control structure design, *Journal of Process Control* (to be submitted).

J. Nandong, Y. Samyudia and M.O. Tadé, Novel PCA-based technique for identification of dominant variables for partial control, *Chemical Product & Process Modeling*, vol. 5 (1), article 7, 2010.

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Nomenclature

Notations

B	Vector of process parameters
D	Vector of disturbance variables
$\Delta F_{D,p}$	Contribution (norm) of dominant variables value to ϕ_p
$\Delta F_{M,p}$	Contribution (norm) of minor variables to ϕ_p
I_{VV}	Variable-Variable Interaction Array or Index
I_{DV}	Dominant Variable Interaction Array or Index
$N_{\Omega_{CS}}$	Total number of the dominant variables corresponding to a vector of performance measures
$N_{U_{mv}}$	Total number of manipulated variables i.e. number of control degree of freedom
U	Vector of input variables
χ	Vector of state variables
X	A matrix of dataset used in the PCA analysis
Y	Vector of output variables

Greek symbols

ϕ_p	Performance measure p
$\Delta\phi_p$	Variation (norm value) of ϕ_p from its steady-state
Φ	Vector of performance measures defining the plant control objectives
$\Delta\Phi$	Vector of variations (norm values) of performance measures
Ω	Vector of dominant variables as in the new partial control context
Ω_p	Set of dominant variables related to ϕ_p
Ψ	Vector of minor variables
Ψ_p	Set of minor variables related to ϕ_p
Σ	Set of input-output variables defining the plant
$\Delta\Phi_{max}$	Vector of maximum allowable variations (norm values) of performance measures

δ_{ij} The value of closeness index of variable y_i in the direction of variable y_j or performance measure \square_j

Abbreviations

CSD	Control Structure Design
CV	Controlled Variable
CI	Closeness Index
DV	Dominant Variable
FOCS	Feedback Optimizing Control Structure
MV	Manipulated Variable
PCA	Principal Component Analysis
PCS	Partial Control Structure
SEIC	Synergistic External-Inherent Control
SOCS	Self Optimizing Control Structure

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1 THESIS OVERVIEW

1.1 Motivation and Objectives

The motivation for this study is driven by two important factors: (1) lack of simple and versatile tool to solve control structure design problem, and (2) lack of research focus to date to address control structure problem in bioprocess systems. With regard to the first motivating factor, it is important to note that the control structure problem is the central issue to be resolved in modern process control. Although research work in this area has spanned more than 3 decades, most of the methods which have emerged over this period are not user friendly (and even impractical) when applied to industrial needs. Thus, further research is required to develop a method which can be easily and effectively put into practice.

Fortunately, a few theoretical frameworks exist within which this complex design problem can be addressed in a systematic way. One of these frameworks is called the Partial Control Structure (Stephanopoulos and Ng 2000), an approach which has been adopted in industry since the inception of modern process control (Tyreus 1999). In this thesis, a new theoretical framework (i.e. refinement of the generalized concept) is established and within which, a new technique based on the principal component analysis (PCA) is developed for implementing the partial control strategy.

As for the second motivating factor, most of the bioprocess control work has focused on the controller algorithm design, which implicitly assumes that controlled variables are pre-determined. In practice, this is not the case where the larger the system of interest, the harder it is to determine the suitable controlled variables. Accordingly, the work described in this thesis aims to fill this research gap where the issues of control structure in bioprocess are addressed in a systematic manner.

The objectives of this study are as following:

- a) Development of a novel technique to implement the partial control strategy (including new theoretical framework of partial control).

- b) Modeling and optimization of the two-stage continuous extractive (TSCE) alcoholic fermentation system.
- c) Design of partial control strategy using a novel technique (developed in (a)) for the TSCE alcoholic fermentation system.

1.2 Novelty, Contributions and Significance

Although the control structure research has spanned over 3 decades, there has been no report in the open literature where the Principal Component Analysis (PCA) is adopted to solving this problem i.e. solving control structure design (CSD) problem based on the plant data analysis. As such, the work in this thesis is the first attempt ever made in the application of PCA to solving control structure problem within the context of partial control concept. The salient feature of the new technique is that, it allows the engineers to implement partial control strategy without the need for rigorous process experience and knowledge. Interestingly, now as then, the implementation of partial control is still made in a rather ad-hoc manner relying heavily on process experience and knowledge.

The technique developed in this PhD work is essentially a fusion of two major concepts known as partial control structure (PCS) and Principal Component Analysis. The adoption of PCS framework is crucial as to provide a theoretical foundation to address the CSD problem. Meanwhile, the PCA is needed to solve the key problem in partial control which is the identification of the so-called *dominant variables*. Note that, we classify this new technique into the *data-oriented approach* implying the incorporation of tool for data analysis e.g. PCA. So in this thesis we refer to this new technique, in general as the *data-oriented approach* and in particular as the *PCA-based technique* (to specifically denote the application of PCA). It is important to note that, most of the mainstream CSD methods fall into two major categories, which are *mathematical-oriented* and *heuristic-hierarchical* approaches. Obviously, the data-oriented approach described in this thesis represents a significant departure from these two mainstream approaches.

In addition, in this work we also address the control structure problem in bioprocess (case study) which has received very little attention to date. Note that, the bulk majority of bioprocess control research in the last 3 decades has focused on the controller

algorithms design and its applications, thus leaving the issue of CSD (in bioprocess) relatively untouched.

The key contributions of the PhD work described in this thesis can be summarized as follow:

1. Development of a novel PCA-based technique for the identification of dominant variables for partial control. Various criteria, conditions and quantitative tools are established, which form the backbone of the PCA-based technique (Chapter 3).
2. Refinement of the partial control concept where a new framework is proposed within which one can clearly define the dominant variable i.e. the dominant variable has not been formally defined before (Chapter 3).
3. Development of a new methodology based on the PCA-based technique for complete partial control design, which incorporates inventory and constraint control objectives. Such methodology for partial control implementation has never been proposed or reported in open literature (Chapter 4).
4. Establishment of new framework for the dynamic controllability analysis which combines the concepts of control relevant metric (v-gap), factorial design of experiment and multi-objective optimization (Chapter 5).
5. Dynamic modeling, optimization and controllability analysis of the two-stage continuous extractive (TSCE) alcoholic fermentation system. Note that, this work is the extension to a single-stage design reported in literature i.e. two-stage design has not been studied before (Chapter 5).
6. Study of control structure design of a typical industrial bioprocess using TSCE alcoholic fermentation system as a case study. Based on this study, a few new insights are obtained such as:
 - a) Change in the nature of variables interaction before (open-loop) and after the control system implementation (closed-loop) can have a significant impact on the dynamic performance of partial control (Chapter 8).
 - b) Non-uniqueness of dominant variable set makes it extremely difficult to solve partial control problem via optimization (Chapter 7).

- c) There should be an optimal size (number of controlled variables) of partial control strategy; otherwise the overall dynamic performance can be degraded by the presence of *bottleneck control-loop* (BCL) (Chapters 6-8).

The significance of this PhD work can be viewed in terms of two key aspects. Firstly, the work provides an effective technique to solving the central issue in modern process control - the control structure problem. Here, the development of new PCA-based technique for implementing partial control strategy allows the use of minimum process experience and knowledge. As this technique is easy to understand, it can greatly facilitate the novices in the implementation of partial control strategy even to the new processes. Note that, previously without any systematic technique it is difficult even for the experienced engineers to implement partial control strategy to a new process, where experience and knowledge about it is still limited.

Secondly, the work shows that one way to improve bioprocess performance is by focusing on the control structure design of the bioprocess plant. In this case, the control structure of the bioprocess control system is more important than the choice of the controller algorithm design. Now it is possible to handle control structure design problem even for a bioprocess (i.e. control structure is normally emphasized in traditional chemical processes), because of the development of PCA-based technique. Additionally, addressing the bioprocess control design within the context of partial control has an advantage because it can lead to a simple and cost-effective control system i.e. small size control system and possibly using only simple PID controllers.

Another aspect which is worthy of consideration is that, this work can serve as a *starting* platform for addressing the multi-scale control structure problem in future. It is interesting to note that especially in bioprocess, because of the increasing trend of integration among multi-scale systems including the microbial system (which is characterized by multi-scale processes from genome to metabolome), the questions which variables to control, which variables to manipulate and how to connect between these two sets will become even more important in future.

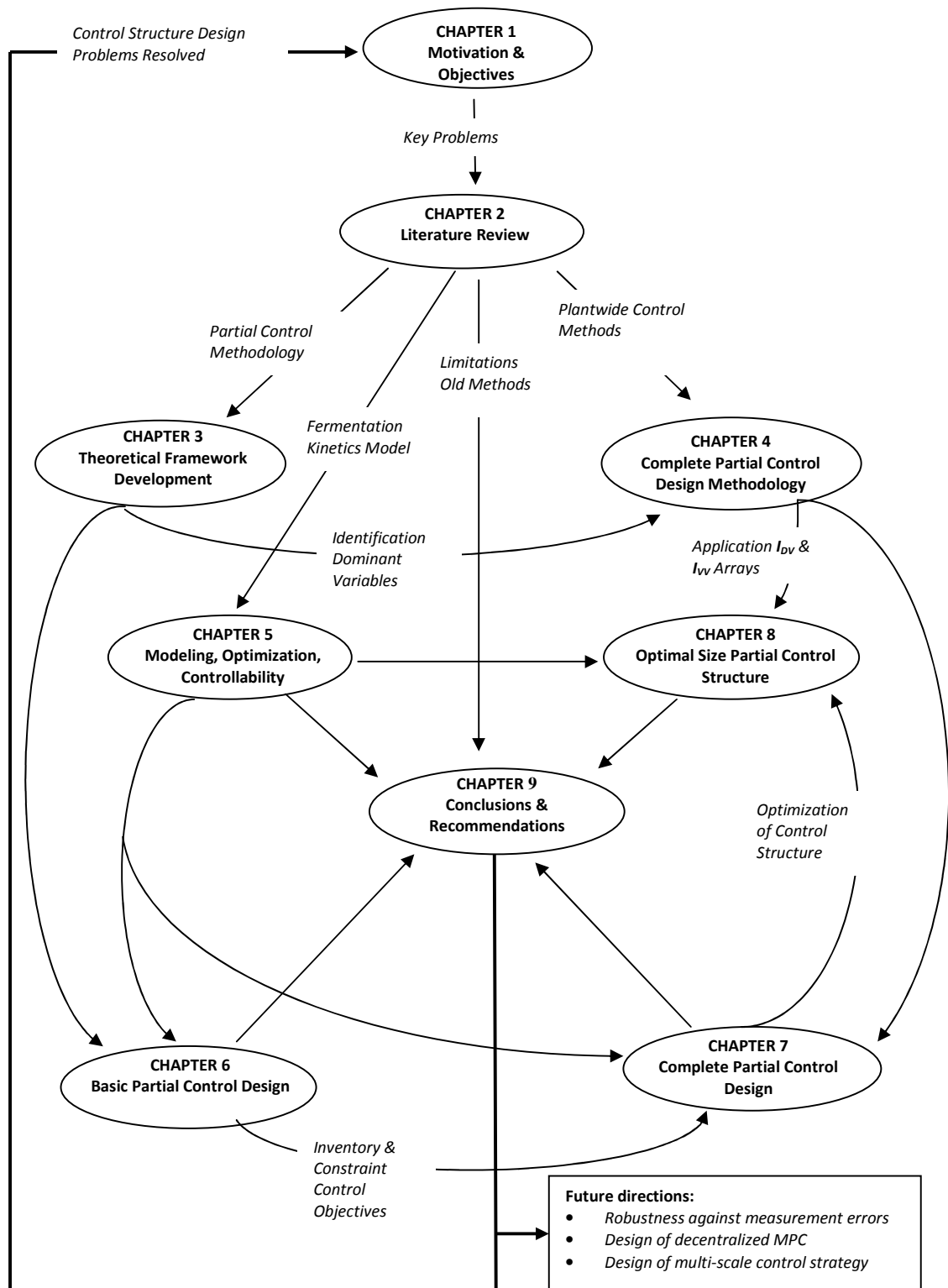


Figure 1-1: Thesis structure overview

1.3 Thesis Structure

Figure 1-1 shows the overview of thesis structure. In summary, this thesis is structured as follows:

Chapter 2 – This covers the literature reviews on the backgrounds relevant to this PhD work, and which are divided into two main parts. The first part deals with the control structure design problem where various methods developed for dealing with this problem are reviewed. Also advantages and limitations of the existing methods are highlighted and the unresolved challenges especially in the area of partial control are identified. One of the key challenges in partial control application arises from its heavy reliance on process experience and knowledge i.e. it is heuristic-based. Thus, if a technique exists to reduce this heavy reliance, then arguably partial control framework can provide effective solution to solving the complex control structure problem. The second part of the review describes the introduction into the bioprocess modeling and control in general. Here, the prevalent approach in bioprocess control design is described and the remaining gaps for further research are identified. One of the gaps is the lack of current research focus on addressing the control structure design in bioprocess control - existing approaches focus heavily on the controller algorithms design. In addition, a review on the extractive alcoholic fermentation technique for the production of fuel ethanol is also presented as to give sufficient background for the bioprocess case study adopted in this thesis.

Chapter 3 – In this chapter, a generalized (classical) concept of partial control structure is presented and its key limitations are further discussed. A new theoretical framework for partial control which can overcome these limitations is developed. Within this new framework, the concept of dominant variables is clearly defined and procedure for identifying these variables via Principal Component Analysis (PCA) is established. In conjunction with the identification of dominant variables via PCA, criteria and conditions are proposed to ensure systematic and consistent result can be obtained. Furthermore, two measures are defined which are called the closeness index (CI) and dominant variable interaction index or array (I_{DV}). The significances of these indices are that, while CI can be used to rank the impact of dominant variables on a performance measure, I_{DV} can be employed to decide on the number of dominant variables, which

must be controlled to ensure acceptable variation in a performance measure. In other word, there is no need to control all of the dominant variables because the interaction among them, makes it possible that controlling only a few of them will indirectly and naturally control other variables. Part of the results regarding the theoretical development is published in Chemical Product and Process Modeling Journal. But it is important to remember that, the theoretical development described in this chapter emerges from the crystallization of several preliminary works, which have been presented in a number of conferences.

Chapter 4 – Here, a methodology for complete partial control design which includes the inventory and constraint control objectives is proposed. It is interesting to note that, the methodology adopts the PCA-based technique developed in Chapter 3 to identify the dominant variables. As to avoid confusion arising from the vast array of objectives that a control system needs to achieve, these objectives are partitioned into 3 major categories as (1) overall control objectives, (2) constraint control objectives, and (3) inventory control objectives. The subset of dominant variables which must be controlled to achieve the overall objectives is termed as the primary controlled variables. Meanwhile both of constraint and inventory control objectives are achieved by controlling subsets of constraint and inventory variables respectively. Here, the applications of PCA-based technique together with the unit operation knowledge allow one to identify which constraint and inventory variables that must be controlled. In other words, just like in the case of dominant variables, there is no need to control all of the inventory and constraint variables because of the existence of variables interaction.

Chapter 5 – Nonlinear dynamic modeling of the case study process called the two-stage continuous extractive (TSCE) alcoholic fermentation system is presented. It is then followed by the optimization of operating conditions of this case study process. Note that, the ethanol yield and productivity are the two key performance measures for this process. Interestingly, these performance measures exhibit opposite trends where the conditions that increase the yield tend to decrease the productivity, and vice versa. Thus, the optimization in this case attempts to find the operating conditions which give the optimal trade-off between these two performance measures. It is also important to highlight in this chapter that a new dynamic controllability analysis framework, which is

based on the combination of concepts of control-relevant metric, factorial design of experiment and multi-objective optimization is proposed. Using the proposed framework, the dynamic controllability of the two-stage design (case study) and single-stage design (reported in literature) of extractive alcoholic fermentation systems is analyzed. Additionally, the optimization of operating conditions and dynamic controllability of the two-stage and single-stage designs are compared.

Chapter 6 – The overall aim of this chapter is to develop a basic partial control strategy for the TSCE alcoholic fermentation system (Chapter 5), which does not directly incorporate the constraint and inventory control objectives. Moreover, as far as the basic partial control strategy is concerned, only the dominant variables are controlled to setpoints with the main emphasis to achieve the specified overall performance measures. In this case, the performance measures are the ethanol yield, percentage conversion of substrate to ethanol and volumetric productivity of ethanol. The values obtained in the optimization of the case study process described in the Chapter 5 are adopted in the simulation of basic partial control strategy. Note that, this is the first chapter in which the PCA-based technique developed in Chapter 3 is used to obtain the dominant variables corresponding to the yield, conversion and productivity. Because the focus is on the basic partial control design, thus the methodology proposed in Chapter 4 is only partially required in this case. Based on the PCA-based technique, this basic partial control design only requires two controlled variables from the four dominant variables identified. Despite its simplicity, the dynamic simulation study shows that the basic partial control design performs satisfactorily well, in term of its ability to maintain the steady-state variations (offsets) of the performance measures within the specified bound. However, the basic design shows rather poor performance in terms of meeting the constraint and inventory control objectives; the constraint and inventory variables show large peaks during the transient response.

Chapter 7 – In this chapter, the proposed methodology for complete partial control design (Chapter 4), which incorporates the constraint and inventory control objectives, is applied to the previous TSCE alcoholic fermentation system mentioned in Chapters 5 and 6. Furthermore, the applications of closeness index and dominant variable interaction index previously described in Chapter 3 are also demonstrated in this chapter.

Dynamic simulation is performed to assess the comparative performances of complete partial control design with and without the PID enhancement technique. Additionally, the impact of control structure on the nature of variables interaction before (open-loop) and after the implementation of a chosen control strategy (closed-loop) is highlighted. Other important aspects pertaining to the partial control are also discussed, which include the working principle of partial control, non-uniqueness of dominant variable set from the classical concept of partial control perspective, and the tool for understanding the variables interaction.

Chapter 8 – An important question from Chapter 7 is how significance is the impact of the variables interaction (which depends on the control structure) on the overall closed-loop performance? This chapter is mainly dedicated to answering this question. Here, a term called *Bottleneck Control-Loop* (BCL) is introduced which in this thesis is referred to as one of the factors that can limit the performance of a control strategy. It is argued in this chapter that, a significant improvement in control (dynamic) performance can be achieved if the BCL can be identified and removed (i.e. size reduction can lead to improvement). However removal of the BCL implies removal of one controlled variable. Thus, while removing the BCL can lead to improved dynamic performance, it can also lead to the degradation in the steady-state performance if the controlled variable being removed is a primary (dominant) variable. In order to assess whether the BCL should be removed or not, the dominant variable interaction index can be used to assess how severe is the penalty on the steady-state performance. The bottom-line is that, there should be an optimal size for the partial control design of a particular system, where too many control-loops (controlled variables) can lead to poor performance.

Chapter 9 – In this chapter, important conclusions that can be drawn from this PhD work are forged into a brief essay. Additionally future works are suggested for improving the current data-oriented approach, and for extending its applications into different areas such as, multi-scale control structure design and design of decentralized model predictive control (MPC) system.

2 LITERATURE REVIEW

2.1 Control Structure Problem

Figure 2-1 depicts the plantwide control problem which can be divided into two main categories as:

- i. Control structure design (CSD) problem.
- ii. Controller algorithm design (CAD) problem.

Despite the great significance of the first category of the problem, the vast majority of the research work has been focusing on the second category of the problem, which assumed that the controlled variables were pre-determined. With regard to the second category of the problem, most of the work has typically dealt with the controller algorithms design and analysis, for instances, the designs of multi-loop PID, nonlinear controller, robust controller and model predictive control (MPC).

Initially, the challenge of plantwide control problem was seriously addressed by (Buckley 1964) in 1960s, where he proposed the concept of dynamic process control in order to handle the problem. While this concept provides practicable solution to the problem, its shortcoming lies in its inability to highlight the *essence* of the control structure problem.

The essence of control structure problem was finely articulated by Foss (1973) in his paper “Critique of Chemical Process Control Theory”, who stated that:

“Perhaps the central issue to be resolved by the new theories of chemical process control is the determination of control system structure. Practicable solutions to this problem are not directly forthcoming from the current methods... it is a formidable task to separate from among these those that should be measured and manipulated and to determine the control connection among them... Such are the questions that need answers, and it is the burden of the new theories to invent ways both of asking and answering the questions in an efficient and organized manner.”

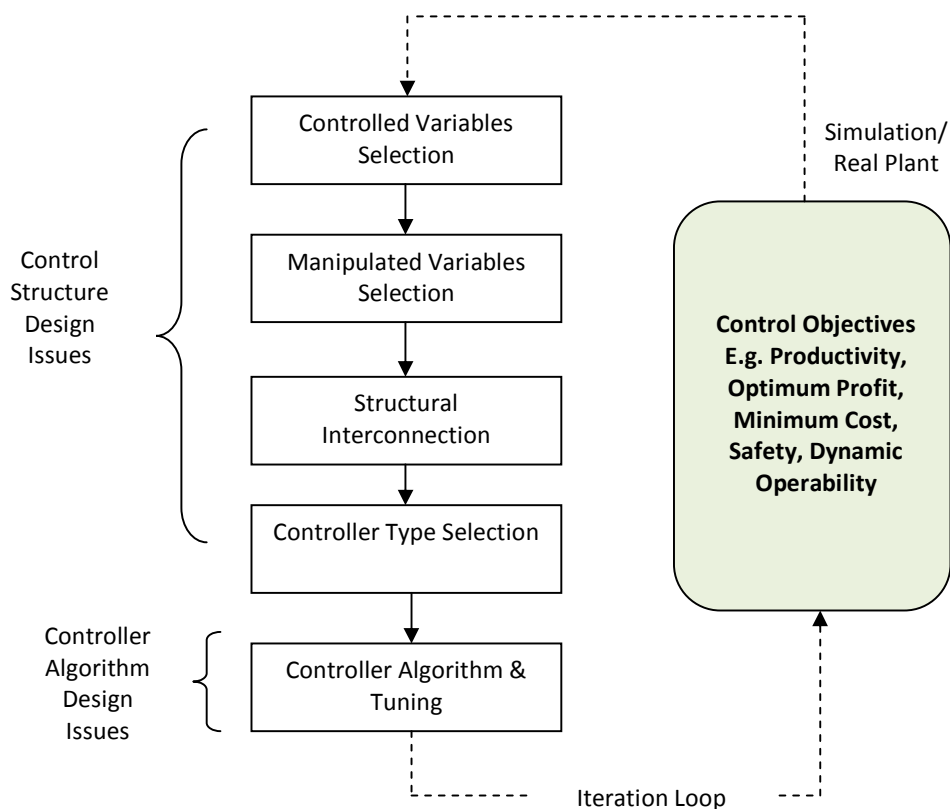


Figure 2-1: Illustration of plantwide control problem

Obviously, the key tasks in CSD are the selections of measured, controlled and manipulated variables, as well as the determination of the structure interconnecting the controlled and manipulated variable sets. These are formidable tasks because the problem is normally open-ended and combinatorial in nature. Thus, no single unique solution exists for a typical chemical process. Very often engineers are just contented with a *workable* control structure that provides satisfactory performance, as it is extremely difficult to identify the *best* one among the ‘sea’ of candidate control structures.

Currently there are 2 major approaches to addressing the CSD problem as follow:

- i. Mathematical-based approach (with optimization).
- ii. Heuristic-hierarchical approaches.

Mathematical based approach relies heavily on the optimization and system theory, for examples, the Feedback Optimizing Control Structure (Morari, Stephanopoulos and Arkun 1980) and its variant the Self Optimizing Control Structure (Skogestad 2000).

Heuristic-hierarchical approach relies heavily on the process knowledge and experience and there are several well-known methods within this family. Among the heuristic methods are the nine-step procedure (Luyben, Tyreus and Luyben 1997), five-tiered procedure (Price and Georgakis 1993) and partial control structure (Shinnar 1981). Some methods also combine the heuristic rules with the decomposition idea of (Douglas 1988), for example, the plantwide control method described in (Zheng, Mahajanam and Douglas 1999). In some articles, the heuristic-hierarchical approach is called the *process oriented approach* e.g. in (Larsson and Skogestad 2000).

Statistical data-oriented approach relies on the availability of plant data and the statistical technique to extract the information from the data. This is an unexplored opportunity since the inception of dynamic process control idea nearly four decades ago. The proposed PCA-based method in this thesis (Nandong, Samyudia and Tade 2010b) is the first reported method within this category. This PCA-based method adopts the framework of partial control in order to address the control structure problem.

Control structure problem is a typical open-ended type of problem and combinatorial in nature. The number of control structure candidates (or input-output structures) can be determined based on (Van de Wal and De Jager 2001) as:

$$N_{IO} = (2^{N_u} - 1)(2^{N_y} - 1) + 1 \quad 2-1$$

Where N_u and N_y is number of manipulated inputs (input degree of freedom) and number of output variables respectively.

Traditionally the plantwide control problem has been addressed based on the unit operation approach (Luyben, Tyreus and Luyben 1997). The basic assumption underlying this approach is that the unit control systems can comprise the entire plant control system in a linear manner – ignores the effect of interaction among the interlinked units.

Because the control structure problem is open-ended in nature, it is important that the problem is addressed in systematic manner. To address this problem in a theoretically-founded manner, formal frameworks are required where (Stephanopoulos and Ng 2000) suggested three choices of formal frameworks as:

1. Feedback optimizing control structure (FOCS)

2. Self-optimizing control structure (SOCS)
3. Partial control structure (PCS)

It should be remembered that unlike the mathematical approach, heuristic-hierarchical approach does not have (or lack of) sound theoretical foundation. Some authors have argued that this is the main reason why the application of heuristic-hierarchical methods often leads to ad-hoc procedures in solving the control structure problem. Surprisingly, despite this limitation, the heuristic-hierarchical approach has received better acceptance than that of mathematical approach in process industry. One of its main strengths is its simplicity as compared to mathematical approach which requires extensive mathematical formulation.

2.1.1 Research Progress in Control Structure Design

Research study on control structure problem has spanned more than 3 decades and where various methods have been developed along the way. Table 2-1 shows the methods which can be categorized into mathematical-based approach. And Table 2-2 shows the methods which are based on either hierarchical or heuristic or combination of both ideas – heuristic-hierarchical approach. Additionally, Table 2-3 shows the methods which can neither be strictly categorized into the mathematical-based nor heuristic-hierarchical approach. These methods normally are hybrid of mathematical, heuristic and hierarchical ideas in various proportions.

While the key advantage of mathematical approach lies in its theoretical foundation which enables engineers to address the CSD problem in a systematic manner, the key advantage of hierarchical approach rests on its simplicity. Because of its theoretical foundation, the mathematical approach allows the translation of the overall operating objectives (normally implicit function of process variables) into a set of controlled variables – this is considered the heart of CSD problem. On the contrary, the heuristic-hierarchical approach is incapable of handling this problem because of its lack of theoretical foundation (Stephanopoulos and Ng 2000).

An ideal approach for control structure problem should unify the advantages of both mathematical and heuristic-hierarchical approaches. Furthermore, it must be able to overcome the limitations faced by both approaches.

Table 2-1: Mathematical and optimization based methods for CSD

Methods/References	Remarks
Feedback Optimizing Control Structure (Morari, Stephanopoulos and Arkun 1980)	<p>Assumes set of controlled variables used in feedback control, which can self-optimize the economic in the presence of disturbances. Provides theoretical framework to address CSD problem and free of engineering heuristics.</p> <p><i>Limitation:</i> (1) Difficult to deal with the multi objectives optimization formulation, (2) heavy computational requirement.</p>
Self-optimizing Control Structure (Skogestad 2000), (Larsson, et al. 2001), (Araujo, Govatsmark and Skogestad 2007)	<p>A variant of feedback-optimizing control structure using single-objective optimization formulation. Key idea is to find a set of variables to control that will lead to <i>acceptable loss</i> in optimum economic performance in the presence of disturbances.</p> <p><i>Applications:</i> Tennessee Eastman (TE) process and HDA plant.</p>
Optimal Control based Approach (Robinson, et al. 2001)	<p>Optimal controller gain matrix is divided into feedback and feedforward parts. Indicates if MPC is preferred over a decentralized plantwide control.</p> <p><i>Limitation:</i> Not clear how controlled variables are selected.</p> <p><i>Application:</i> Reactor with recycle and polymerization process.</p>
MILP Optimization based on Dynamic Model (Wang and McAvoy 2001)	<p>Adopts MILP optimization to synthesize plantwide controller in three stages as fast and slow safety variables and followed by product variables.</p> <p><i>Limitation:</i> Not clear how controlled variables are selected.</p> <p><i>Application:</i> TE process</p>
MILP Optimization based on Linear Dynamic Economics (Narraway and Perkins 1993), (Kookos and Perkins 2002)	<p>Address how changes in control structure alter the economics. Requires linear dynamic economics model.</p> <p><i>Application:</i> Reactor/separator process and double effects evaporator system.</p>
Heuristic-Optimization Method (Kookos and Perkins 2001)	<p>Heuristic rules are incorporated into the MILP optimization formulation. Heuristics are used for <i>quick generation</i> of promising control structures.</p> <p><i>Application:</i> Double-effects evaporator, HDA plant and TE process</p>

Table 2-2: Heuristics-Hierarchical based methods for CSD

Methods/References	Remarks
Dynamic Process Control (Buckley 1964)	Divides CSD problem based on time scales: (a) material balance – slow scale, and (b) quality – fast scale. Provides practical solution to CSD problem. Many heuristic methods that follow still inherit the characteristics of this method.
Cause-and-Effect Representation (Govind and Powers 1982)	Use simple input-output models to generate alternate control structures. First non-numerical problem-solving technique to synthesize control structure.
Partial Control based on Engineering Experience (Shinnar 1981), (Arbel, Rinard and Shinnar 1996)	Provides theoretical-founded way to address CSD problem. Key idea is to control a small subset of variables known as dominant variables, which will lead to acceptable variations in operating objectives. <i>Limitation:</i> Difficulty in identifying suitable dominant variables via engineering experience and process knowledge. <i>Application:</i> Fluidized Catalytic Cracker (FCC)
Partial Control based on Thermodynamics (Tyreus 1999a), (Tyreus 1999b)	Using expressions derived from thermodynamic knowledge to determine suitable dominant variables. <i>Application:</i> TE process
Five-tiered Framework (Price and Georgakis 1993)	Five tiers: (1) production rate control, (2) inventory control, (3) product specification control, (4) equipment & operating constraints, and (5) economic performance enhancement. <i>Application:</i> Reactor/separator system
Nine-step Procedures (Luyben, Tyreus and Luyben 1997)	Establish: (1) control objectives, (2) degree of freedom, (3) energy management system, (4) production rate, (5) product quality, safety, operational & environmental constraints control, (6) inventories control, (7) component balances consistency, (8) individual unit operation control, and (9) improve dynamic controllability. <i>Application:</i> TE and HDA processes.
Heuristic-Simulation Framework (Konda, Rangaiah and Krishnaswamy 2005)	Simulation is combined with nine-step procedure facilitating the novices to use the heuristic method. <i>Application:</i> HDA process

Table 2-3: Other methods for CSD

Research Work/Reference	Remarks
Hierarchical Approach (Douglas 1988), (Zheng, Mahajanam and Douglas 1999)	<p>Use Douglass (1988) idea of hierarchical decomposition based on economics. Simple modifications can be used to determine the optimum surge capacities of a process. Framework can be used to integrate process design and control.</p> <p><i>Limitation:</i> Can lead to conflicting results.</p> <p><i>Application:</i> Reactor/separator system.</p>
Balanced Scheme Control Structure (Wu and Yu 1996)	<p>Emphasizes the use of balance control scheme between units e.g. reactor and separator to handle large load changes.</p> <p><i>Application:</i> Reactor/separator process.</p>
Decision-based Approach (Vasbinder and Hoo 2003)	<p>Uses analytic hierarchical process to prioritize the various objectives. Plant is decomposed, and for each module the nine-step approach is invoked to design the control structure.</p> <p><i>Application:</i> Reactor/separator process.</p>
Thermodynamic Approach (Antelo, Muras, et al. 2007)	<p>Combined concept of process networks, thermodynamics and systems theory to derive robust decentralized controllers that ensure plant stability.</p> <p><i>Limitation:</i> Can be too complicated for large-scale system.</p> <p><i>Application:</i> CSTR</p>
Control-relevant Metric Approach (Samyudia, et al. 1995)	<p>Framework based on control relevant metric is used to screen alternative control structures, with emphasis on stability and achievable performance of the system under decentralized control architecture. The method does not provide way to select controlled variables.</p> <p><i>Limitation:</i> Not clear how controlled variables are selected.</p> <p><i>Application:</i> Reactor/separator process.</p>

2.1.2 Partial Control Structure

Early motivation for the applications of partial control arises from the technology limitations and cost factors, which necessitates the use of a few simple measurements and actuators to control the process (Tyreus 1999a). Despite the rapid advancement in technology today, partial control remains an important control strategy in process industries. This is due to the limited number of available manipulated variables normally encountered in real cases i.e. the number of manipulated variables is normally smaller than the number of output variables - *thin* plant cases.

The subset of variables which are controlled at constant values such that, the variations in the operating objectives are acceptable in the face of external disturbance occurrence is called the *dominant variables*. It is important to note that, the heart of partial control problem lies in the identification of these dominant variables. From its early inception, in partial control the search for the dominant variables has been based on extensive engineering experience and process knowledge i.e. by heuristic approach. Tyreus (1999a) proposed a systematic approach (albeit with restricted applications) to identify the dominant variables but requires thermodynamics knowledge of the process. One limitation of this method, however, it is only suitable for finding variables which have strong thermodynamic relationship with the operating objectives; otherwise, if the operating objectives are not strongly related to thermodynamic, then this method will not work. Other than this thermodynamic approach which has narrow application restricted by the thermodynamic knowledge, unfortunately, there has been very little progress in the development of other systematic approach to identify the dominant variables.

The applications of partial control to fluidized catalytic cracker and Tennessee Eastman Process were reported by (Arbel, Rinard and Shinnar 1996) and (Tyreus 1999b) respectively. Note that, the Tennessee Eastman Process has also been adopted as a case study for testing other CSD methodologies, for examples, the combined method based on steady-state analysis, engineering judgment and simulation (McAvoy and Ye 1994), hierarchical procedure based on thermodynamics (Antelo, Banga and Alonso 2008) and Self Optimizing Control Structure (Larsson, et al. 2001).

Partial control framework offers an advantage over the heuristic approach in term of its ability to address the control structure problem in a systematic manner – i.e. it has

sound theoretical framework. However, the key challenge in partial control currently lies in the difficulty to identify the dominant variables. A framework for defining the partial control problem was proposed by (Kothare, et al. 2000), which allows the incorporation of both engineering-based decisions and more rigorous theoretical tools to achieve the goals of partial control. Nevertheless, this framework does not provide an efficient tool to identify the dominant variables. More detail regarding partial control will be dealt with in Chapter 3.

2.2 Bioprocess Modelling and Control

2.2.1 Introduction

Biotechnology is the oldest known technology which has served the humanity since pre-biblical times (Demain 1981) where one of its earliest applications is to produce beer by fermentation. Undoubtedly, biotechnology is one of the most important processes in nature which is inherently multi-scale in character (Ayton, Noid and Voth 2007). Other well-known examples of important processes which are multi-scale include turbulent flows, mass distribution in the universe and vortical structures on the weather map. An important feature of multi-scale processes is that different physical laws may be required to describe the systems involved on different scale (Weinan and Engquist 2003).

The incorporation of multi-scale knowledge in the process modelling is not straightforward (Stephanopoulos, Dyer and Karsligil 1997, Bassingthwaight, Chizeck and Atlas 2006). Consequently, despite the well-known multi-scale nature of systems involving industrial microbes, the analysis and design approaches adopted in the bioprocesses are still largely based on the simplified macro-scale concept. This macro-scale approach is also known as *formal* approach (Moser 1984). The key feature of this formal approach is that the detailed phenomena occurring at the fine scales (i.e. fine details) are generally ignored. Based on this approach, the fine-scale phenomena (i.e. detailed cellular metabolism) such as those occurring at the cellular level are lumped into macro-scale parameters, for examples, specific growth and product formation rates and yield coefficients. The primary motivation for adopting this approach rests on its

simplicity and practicality in the absence of detailed information and knowledge particularly on the fine resolutions.

2.2.2 Bioreactor: Definition of Performance and Research Focus

At the heart of a bioprocess is the bioreactor which has been considered to provide a central link between the starting feedstock and the product. As such, it plays a critical role in the economics of biotechnological processes in general (Cooney 1983).

The bioreactor must be designed to meet the specific needs and constraints of a particular process, and its design will normally affect both cost and quality of the final product or service. Therefore, the practicality of the bioreactor performance is essentially determined by the benefit/cost ratio (Lubbert and Jorgensen 2001). With respect to the benefit, it is defined in terms of the amount of the desired product produced and its market price. On the other hand, the cost reduction is the major objective in biochemical engineering. In a nutshell, the bioreactor performance encompasses all activities undertaken to ensure reproducible operation or to improve the performance of biochemical conversion step of the bioprocess system.

Research efforts for improving the performance of bioreactor could be broadly divided into two important aspects:

- a) Key enabling tools.
- b) Biosystem improvement.

Furthermore, there are two major key enabling tools which support the research efforts for improving the bioreactor performance which are:

- a) modelling, computation and analysis.
- b) Measurement technology including the sampling, analytical techniques and sensors development.

Meanwhile within the biosystem improvement efforts, one could further divide the key research works into two main categories as:

- a) Bioreactor design and operation.
- b) Microbial strain improvements or cellular system improvement.

Figure 2-2 Framework of relationship between the research on key enabling tools (modelling and measurement technology) with the research on bioreactor design and operation towards the improvement of bioreactor performance

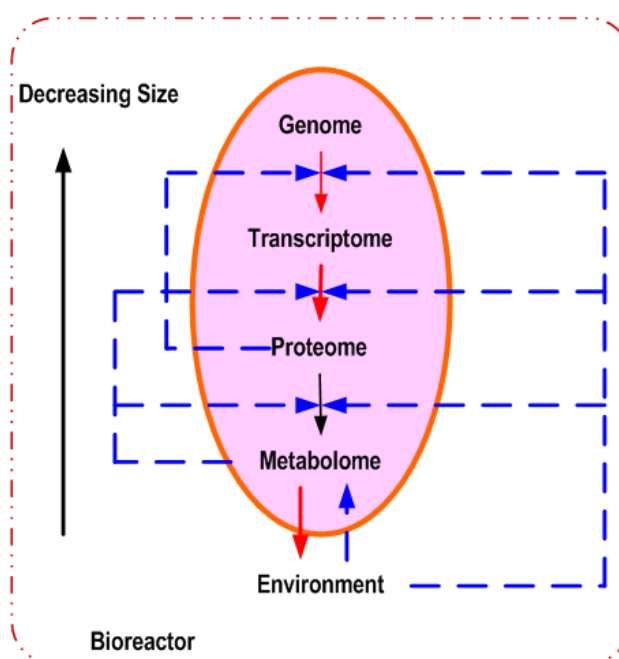


Figure 2-3: Schematic representation of interactions between the cellular and environment and the cellular metabolism. The biochemical synthetic route from genome to the metabolome is shown as unbroken arrows. Possible interactions in that route (e.g. transcription factors or effectors binding to the genome, enzymatic feed-back loops, or poisoning effects) are shown by dashed arrows (Liden 2002)

Figure 2-2 shows an overview of these key research areas across different scales (cellular up to bioreactor level), which are vital towards the improvement of bioreactor (benefit/cost ratio) performance, and hence could lead to an overall improvement of the biotechnological process. Note that, the progress in measurement technology has allowed better access to detailed measurements such as the cellular metabolites concentrations, intracellular fluxes and cellular physiological states. This in turn creates large volume of multi-scale data and information about the overall bioreactor system ranging from the genome scale, to metabolome and up to the macro-scale level of bioreactor.

The multi-scale nature of the overall bioreactor system can be illustrated by Figure 2-3. One of the major research efforts in recent years are to interpret and evaluate this large volume of data or information through the application of modelling technique. In connection to such efforts, the progress in modelling could also be viewed as a mean to create valuable *new insights* about the biosystem of interest and to provide new research directions for further improvement (see Figure 2-2).

2.2.3 Key Challenges in Bioprocess Design and Operation

Table 2-4 summarizes the key challenges (Cooney 1983, Liden 2002) in bioprocess design and operation, which in turn frequently put a limit on the bioreactor practical performance as measured by the benefit/cost ratio. Voluminous research efforts have been dedicated in the last 30 years in order to overcome these key challenges mainly through the applications of process system engineering concept to the bioreactor design and operation and more recently through the concept of metabolic engineering to improve the microbial strain of interest.

In this review, one of the aims is to present how these key challenges have been addressed from modelling, design and control point of views using alcoholic fermentation process as a case study. Following this review, another important aim is to highlight the key research gaps which become the basis of this PhD study.

Table 2-4: Key challenges in bioreactor design and operation

Challenges	Remarks
Limitation on heat and mass transfer	Particularly critical for aerobic fermentation, immobilized cells and heavy cells density fermentations.
Low volumetric productivity	Due to (1) low biocatalyst activity, (2) inhibitory effects (product, high substrate concentration, temperature).
Low final product concentration	Causes high recovery costs.
High product quality requirement	Important to minimize the by-product formation & thus increase the yield of desired product.
Lack of physiological understanding	Complex physiology prevents effective use of measured variables to design control system for controlling the culture.
Lack of sensors to measure primary variables	Primary variables are substrates, products and biomass concentrations.
Limited number of suitable manipulated variables	Use of different fermentation system designs to increase number of inputs.

2.2.4 Modelling of Fermentation Process

In process engineering the use of model to represent the key dynamic behaviours of the process of interest is a prevalent practice. With respect to biochemical engineering, there are four key reasons why models are necessary (Bailey 1998):

1. To think (and calculate) logically about what components and interactions are important in a complex system i.e. from DNA sequence to phenotype.
2. To discover new strategies.
3. To make important corrections in the conventional wisdom.
4. To understand the essential, qualitative features.

The key reason for making models is to be able to bring measure of order to our experience and observations (data and information), as well as to make specific predictions about certain aspects of the world we experience (Casti 1992). Therefore, mathematical modelling does not make sense without defining, before making the model, what its use is and what problem it is intended to help to solve – aim and scope of the model development. In bioprocess modelling, the key challenge is to transfer and adapt the developed modelling methodology from technical to biological systems, where the extent of applicability remains open due to several substantial differences between the two systems (Wiechert 2002).

Furthermore, the aim and scope of modelling applications can be summarized into six important categories (Wiechert 2002) as:

- 1) **Structural understanding** – the model is mainly used to help focusing the attention on what is considered the essential parts of the system.
- 2) **Exploratory simulation** – the most frequent application of models is the exploration of the possible behaviour of a system. The model might be very crude, but could help to achieve a rough understanding of the system behaviour and to reject false hypotheses.
- 3) **Interpretation and evaluation of measured data** – the reproduction of experimental data by mathematical models is a well-established tool in all scientific disciplines. It is very important to point out that in most cases this is merely a reproduction of measured data i.e. does not mean it even has any predictive power.

- 4) **System analysis** – the models could be used to help in obtaining better understanding of the system's structure and its qualitative behaviour, e.g. identification of functional units in metabolic and genetic systems.
- 5) **Prediction and design** – the validated model could be used to predict the outcome of future experiments. However, the predictive power is often restricted to a narrow scope that does not always contain intended target configurations or ranges of conditions.
- 6) **Optimization** – the application of models in engineering disciplines is the state of the art, but application to biotechnological systems may not be straight forward.

In the modelling of bioprocess, the key aspect is how to capture the key behaviours of the cell populations. Figure 2-4 illustrates the classification of mathematical and other representations of cell populations as introduced by Fredrickson (Bailey 1998). Fredrickson introduced the term “segregated”, to indicate explicit accounting for the presence of heterogeneous individuals in a population of cells. And, the term “structured”, is designated for the formulation of model in which cell material is composed of multiple of chemical components. Most models and measurements belong to the nonsegregated class.

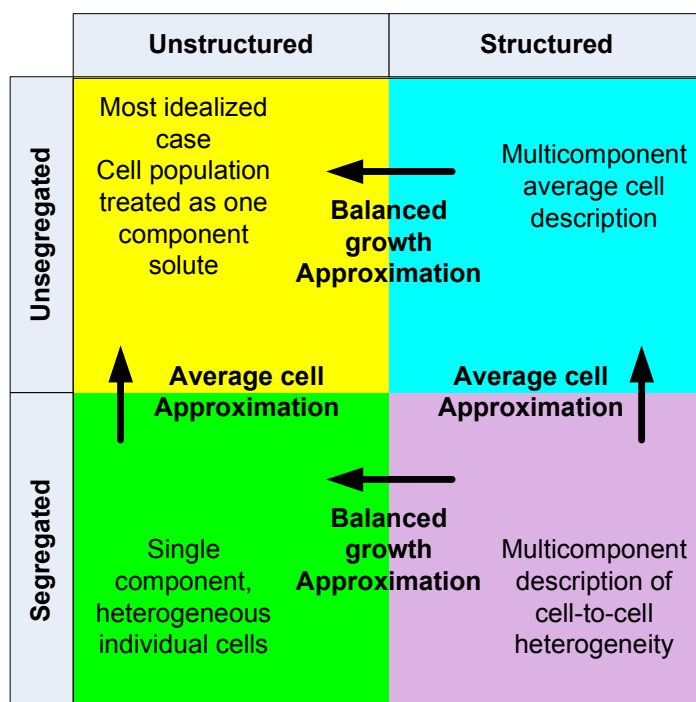


Figure 2-4: Classifications introduced by A.G. Fredrickson for mathematical (and other) representation of cell populations (Bailey 1998)

Table 2-5 summarizes the key behaviours of alcoholic fermentation process which have been the subject of extensive modelling efforts i.e. to capture the behaviours in quantitative manners. The development of kinetics models based on Monod type, which embeds the inhibitory effects of high ethanol and substrate concentrations on the specific growth and product formation rates is a common practice in the formal macroscale (or unstructured) approach. Ethanol is considered as the principal stress factor in yeasts during fermentation processes.

Various studies have been dedicated to understand the mechanisms of ethanol inhibitory effects on yeasts (Aguilera, et al. 2006, Alexandre, Rousseaux and Charpentier 1994, D'Amore and Stewart 1987, Jones 1989, Ricci, et al. 2004). A comprehensive review on the kinetics modelling of microbes (both bacteria and fungi) based on structured modelling approach can be found in (Nielsen and Villadsen 1992).

Table 2-5: Modelling of key behaviours in alcoholic fermentation process

Behaviours	Remarks	References
Inhibitory effects due high product or substrate or biomass concentration	Due to high substrate and product concentrations. High biomass concentration causes limitation on mass transfer, and high temperature causes high death rate. Frequently lead to low yield and productivity.	(Ghose and Tyagi 1979), (Luong 1985), (Garro, et al. 1995), (Jarzebski 1992), (Starzak, et al. 1994), (Thatipamala and Hill 1992), (Phisalaphong, Srirattana and Tanthapanichakoon 2006), (Costa, et al. 2001)
Mixed physiological states or <i>Crabtree effect</i> .	At low dilution rate glucose is used oxidatively. At high dilution rates respiro-fermentative occurs even in the presence of excess oxygen.	(Anderson and Von Stockar 1992), (Hanegraaf, Stouthamer and Kooijman 2000), (Thierie 2004)
Oxygen supply or micro-aerobic fermentation	Oxygen supply could increase cell viability and reduce by-products formation such as glycerol.	(Slininger, et al. 1991), (Dellweg, Rizzi and Klein 1989), (Grosz and Stephanopoulos 1990)
Oscillatory phenomenon	Caused by inhibitory action, and negative coupling between product formation and biomass growth	(Jarzebski 1992), (Garhyan and Elnashaie 2004), (Jobses, et al. 1986)
<i>Lag</i> phase and dynamic of the respiratory bottleneck	Adaptive period for cell adjusting from one substrate to another (diauxic lag phase).	(Sonnleitner and Hahnemann 1994), (Sonnleitner, Rothen and Kuriyama 1997), (Pamment, Hall and Barford 1978)
Cellular Metabolism	Modelling to understanding cellular metabolism and physiology. Used to optimize conditions, and in directing genetic changes to produce improved strains.	(Gombert and Nielsen 2000), (Patnaik 2001), (Rizzi, et al. 1997), (Lei, Rotboll and Jorgensen 2001), (Galazzo and Bailey 1990), (Bideaux, et al. 2006); (Steinmeyer and Shuler 1989)

2.2.5 Macro-scale Modelling Approach

Modelling of bioreactor involves 2 major components namely:

- 1) Kinetics model of the microbe being used.
- 2) Mass and energy (sometimes momentum) balances of the bioreactor.

The kinetics model of the microbe can be either in the form of unstructured or structured. Vast majority of models used in the bioreactor modelling, design and optimization is of the unstructured type because of its simplicity.

Figure 2-5 illustrates the idea of macro-scale approach to bioreactor modelling. Here, U_{mac} and Y_{mac} represent the vectors of macro-scale inputs and outputs respectively. The descriptions of the bioprocess in general consists of three sets of equations: (1) process mass conservation equations describe the type of bioreactor, (2) kinetics equations, and (3) yield equations replace the stoichiometry of chemical processes, and describe the relationship between the rates of consumption and product formation (Andrews 1993). Note that, the focus of modelling in macro-scale approach is to capture the macro-scale process behaviours.

2.2.5.1 Bioreactor Modelling

The next set of equations is to describe the bioreactor system through the process mass conservation equations for each components and energy balance. The conventional macro-scale model (Figure 2-5) could in general be represented as a set of differential-algebraic equations (*i.e.* DAEs system) as follows.

First, the set of differential equations representing the bioreactor or macro-scale state variables can be written as:

$$\dot{X}_{mac} = f_{mac}(X_{mac}, U_{mac}, \beta) \quad 2-2$$

Where $X_{mac} \in R^{n_x}$, $U_{mac} \in R^{n_u}$ and $\beta \in R^{n_\beta}$ are vectors of macro-scale state variables, macro-scale input variables and kinetic parameters respectively. Note that, in this case, the kinetic parameters of interest are the growth, product formation and substrate consumption rates. The f_{mac} is generally a nonlinear function of its arguments.



Figure 2-5: Schematic representation of macro-scale modelling approach

Meanwhile the bioreactor output variables can be expressed as:

$$Y_{mac} = h_{mac}(X_{mac}, U_{mac}) \quad 2-3$$

Assuming the time-varying kinetic parameters can be written as:

$$\beta = g_{mac}(X_{mac}) \quad 2-4$$

The dynamic of the parameters in response to the state variables change is assumed instantaneous i.e. follows the dynamic of the macro-scale system. But credible studies show that this might be partially true as cells must somehow sense the changes in the environmental conditions and have a choice to respond, thus introduces certain *lag* time (Sonnleitner 1998) . This actually leads to some finite time, for example, the relaxation time of yeast when subject to excess substrate supply can be on the order of 1 hour (Sonnleitner, Rothen and Kuriyama 1997).

Additionally, Figure 2-5 representation is generally called the *black box* approach. The detailed processes occurring in the cells are ignored and lumped together as the macro-scale parameters β e.g. specific growth rate, specific product formation rate and yield coefficients.

2.2.5.2 Unstructured Fermentation Kinetic Modelling

In this case, we describe the kinetic modelling which is frequently adopted in alcoholic fermentation. There are three types of inhibitory effects, which are frequently encountered in the ethanolic fermentation in particular and other types of fermentation in general, which are:

- 1) Product inhibition e.g. too high ethanol concentration can reduce the growth and product formation rates.

- 2) Substrate inhibition i.e. when the glucose concentration is too high, the growth rate can be significantly reduced.
- 3) Biomass inhibition, i.e. too high the biomass concentration can lead to mass transfer limitation which can reduce the growth and product formation rates.

The substrate limitation based on the *Monod* equation for the specific growth rate can be written as follows:

$$\mu = \mu_0 \frac{S}{K_s + S} \quad 2-5$$

Where S is the substrate concentration and K_s is a parameter. Taking into account the ethanol inhibition effect, we can write the specific growth rate as:

$$\mu = \mu_i \frac{S}{K_s + S} \quad 2-6$$

Where the ethanol concentration (P) inhibitory effect can be expressed in various forms (Luong 1985) such as:

$$\text{Linear Form: } \mu_i = \mu_0 \left(1 - \frac{P}{P_m}\right) \quad 2-7$$

$$\text{Exponential Form: } \mu_i = \mu_0 e^{-K_2 P} \quad 2-8$$

$$\text{Hyperbolic Form: } \mu_i = \mu_0 \left(\frac{1}{1 + P/K_3}\right) \quad 2-9$$

$$\text{Parabolic Form: } \mu_i = \mu_0 \left(1 - \frac{P}{P_m}\right)^n \quad 2-10$$

Moreover, in the case of high cell density fermentation, the inhibitory effect due to the biomass concentration (X_t) on the kinetics needs to be considered. A model which incorporates both ethanol and biomass concentrations (Jarzebski, Malinowski and Goma 1989) can be represented as:

$$\mu_i = \mu_0 \left[1 - \left(\frac{P}{P_m}\right)^A\right] \left[1 - \left(\frac{X_t}{X_m}\right)^B\right] \quad 2-11$$

If the substrate inhibition is assumed to take linear form (Thatipamala and Hill 1992), then the following expression could be adopted:

$$\mu_i = \mu_0 \left(\frac{S_{max} - S}{S_{max} - S_{min}} \right) \quad 2-12$$

Additionally, the combined inhibitory effects of substrate, product and biomass can be expressed as reported in (Costa, et al. 2001):

$$\mu_i = \mu_0 \exp(-K_i S) \left(1 - \frac{X_t}{X_{max}} \right)^m \left(1 - \frac{P}{P_{max}} \right)^n \quad 2-13$$

Furthermore, to take into account the effect of temperature, the parameters μ_0 , K_i , X_{max} and P_{max} can be expressed as functions of temperature T , e.g. $\mu_0 = f_1(T)$, $K_i = f_2(T)$ etc. Next, the rate of biomass growth can be written as:

$$r_x = \mu X_v \quad 2-14$$

Where X_v is normally referred to as the viable cell concentration i.e. to differentiate it from the dead cell concentration X_d . Thus, the total cells concentration $X_t = X_v + X_d$.

It follows that, the growth rate can be linked to the product formation and substrate consumption rates through *yield coefficients*.

Thus, the rate of substrate consumption following the equation of *Pirt* (Garro, et al. 1995):

$$r_s = \frac{r_x}{Y_{X/S}} + m X_v \quad 2-15$$

Here, $Y_{X/S}$ is the yield coefficient of biomass produced per amount of substrate consumed and m is called the maintenance coefficient.

Meanwhile, the rate of product formation could be expressed as *Luedeking-Piret* equation (Garro, et al. 1995):

$$r_p = Y_{P/X} r_x + m_p X_v \quad 2-16$$

Note that, $Y_{P/X}$ is called the yield coefficient of the product produced per amount of biomass produced i.e. this parameter links the growth to product formation. Meanwhile, m_p is the coefficient that relates to the growth-independent product formation by the existing viable cells.

It is interesting to note that, the *kinetics* and *yield* equations are independent of the type of bioreactor. Therefore, the kinetics and yield equations can be combined together

to constitute a *description* of the *metabolism* and how it is affected by the cell's physicochemical environment (Andrews 1993) e.g. substrate and product concentrations.

2.2.6 Multi-scale Modelling Approach

Figure 2-6 illustrates the multi-scale approach to modelling bioreactor (Nandong, Samyudia and Tade 2007). An essential feature distinguishing the multi-scale approach from the traditional macro-scale approach is that in the former, the cellular system is no longer treated as a black box. The U_{mic} , X_{mac} and β are vectors of micro-scale inputs, macro-scale state variables and macro-scale model parameters, respectively.

Multi-scale system consists of both macro- and micro-scales dynamics, where the macro-scale sub-system could generally be expressed as:

$$\dot{X}_{mac} = F_{mac}(X_{mac}, U_{mac}, \beta) \quad 2-17$$

$$Y_{mac} = G_{mac}(X_{mac}, U_{mac}) \quad 2-18$$

Now, the kinetics parameters can be linked with the micro-scale system as follows:

$$\beta = g_{mic}(X_{mac}, X_{mic}) \quad 2-19$$

$$\dot{X}_{mic} = f_{mic}(X_{mac}, X_{mic}, U_{mic}, \gamma) \quad 2-20$$

$$Y_{mic} = g_{mic}(X_{mac}, X_{mic}, U_{mic}) \quad 2-21$$

Where $X_{mic} \in R^{n_{xmic}}$, $U_{mic} \in R^{n_{umic}}$, $Y_{mic} \in R^{n_{ymic}}$ and γ are vectors of micro-scale state variables, input variables, output variables and parameters respectively.

Moreover, Eq. 2-20 implies that the micro-scale parameter γ is a time-varying and a function of the micro-scale state variable, so it can be expressed as:

$$\gamma = h_{mic}(X_{mic}) \quad 2-22$$

Alternatively, rather than computing γ as a function of micro-scale state variables as in Eq. 2-22, the multi-scale model shown in Figure 2-6 could be further extended to accommodate even finer scale (e.g. genome scale). Hence, the parameter γ could be computed as a function of the state variables of this finer scale sub-system.

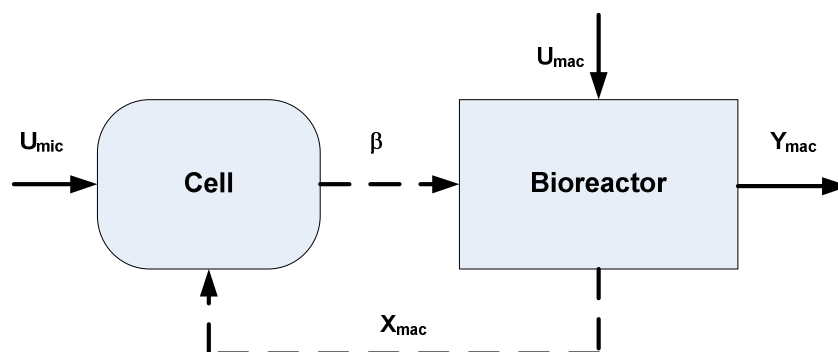


Figure 2-6: Block diagram representation of multi-scale bioreactor system

The multi-scale system shown in Figure 2-6 is typically known as an *embedded* type. For more details and explanation about the classification of multi-scale systems, interested readers could refer to the review by (Ingram, Cameron and Hangos 2004).

It is important to highlight that the parameters β and γ play important role in the multi-scale modelling because they provide the links across the different scales (Sainz, et al. 2003). Indeed one of the key challenges in multi-scale modelling is that, how to link the information across the different scales of time and length (Ingram, Cameron and Hangos 2004).

2.2.7 Fermentation Control and Model Application

Although the simple macro-scale models are often sufficient for process control purposes, there is an increasing need for the models incorporating multi-scale information and knowledge. In general, this is largely due to the motivation to gain better control over chemical reactions, as well as product molecular architecture, conformations and morphology (De Pablo 2005).

Recent increase of trend in the applications of advanced process control (APC) techniques in bioprocess industry has been motivated by the expiration of pharmaceutical patents and continuing development of global competition in biochemical manufacturing (Henson 2006). Notwithstanding these strong motivations, the role of process control in biotechnology industry is still very limited as compared to

that in the petroleum and chemical industries. For instance, the model-based strategies have been scarcely implemented in biological processes (Komives and Parker 2003).

Surprisingly, in the field of monitoring and control, according to (Junker and Wang 2006) fermentation technology is substantially ahead of its sister chemical areas, which are owing to requirements for tight control of cellular biochemical environment in order to optimize yield and productivity. It is important to note that, this view might be based on the level of sophistication of the technologies involved in bioprocess control, which are generally higher than that of chemical process i.e. sophisticated biosensors and complex sampling and analysis techniques, and use of evermore rigorous multi-scale approach.

In contrast, the use of cheap sensors might be sufficient for the chemical processes. In this respect, despite the sophisticated hardware/software application in bioprocess, so far it is the chemical process that is leading in the development of advanced controller algorithms such as robust and nonlinear model predictive controllers. Excellent reviews on the progress in monitoring, modelling and control of bioprocess could be found in (Schugerl 2001) and (Alford 2006).

Just like in chemical processes, the *nonlinearity* in bioprocesses has been considered as one of the key limitations to control performance. Thus, in turn the choice of controller algorithm (e.g. linear PID or nonlinear controller) is critical and could greatly impact the overall bioreactor performance. One reason for this *nonlinearity* is due to the frequent drift in process parameters from that of nominal values particularly when external disturbances occur. To overcome this limitation, various types of controller algorithms have been adopted in bioprocess which in general could be broadly classified as: (a) adaptive control, (b) robust control, and (c) nonlinear model-based control.

2.2.7.1 *Adaptive Control of Fermentation*

With respect to the adaptive control, there are two main reasons for using this technique, which are (a) strong nonlinear and *nonstationary* dynamics of living organisms, and (b) lack of cheap sensors capable of providing on-line measurements of the fermentation parameters (Vigie, et al. 1990). Adaptive control is an approach to dealing with uncertain systems or time-varying systems. This is applied mainly to systems with

known dynamic structure, but *unknown* constant or slowly-varying parameters (Slotine and Li 1991).

It is important to note that, there are various versions of adaptive control for fermentation processes. The key feature differentiating the different versions rests on the various combinations of the basic adaptive control technique with other control techniques such as the optimal, robust and neural network control concepts. For instances, the combined adaptive and optimal control concepts (Ban Impe and Bastin 1995), nonlinear adaptive control (Mailleret, Bernard and Steyer 2004), fuzzy combined adaptive control (Babuska, et al. 2002), neural network and adaptive control (Syu and Chang 1997) and (Renard and Wouwer 2008).

2.2.7.2 *Robust Control of Fermentation*

In view of complex multi-scale nature of bioprocesses, it is very often that the dynamic structure is unknown or poorly understood. Thus in this case, robust control is an appealing alternative in which case the uncertainty in term of plant/model mismatch could be systematically accounted for in the controller algorithm design.

An interesting case is the robust H_∞ multivariable control, which is arguably a promising and preferred model-based, APC strategy if it is desired to maintain both closed-loop stability and achieving specific performance over a range of operating conditions (Lee, Wang and Newell 2004). Some implementation issues of robust control theory to continuous stirred tank bioreactor are presented by (Georgieva and Ignatova 2000). Additionally, robust controller could also be conveniently applied to fed-batch fermentation where minimal process knowledge and minimal measurement information is available (Renard, et al. 2006).

2.2.7.3 *Model-based Control of Fermentation – Application of Macroscale Models*

In the case of adaptive and robust controllers, rather crude model (minimal knowledge) is quite sufficient to design the controller algorithms. However when more rigorous nonlinear model of the process is available, an opportunity exists to use the so-called

model based controllers. One of the most attractive techniques developed in chemical process applications is the nonlinear model predictive controller (NMPC).

The key advantage of NMPC other than its natural ability to consider process nonlinearity is its ability to handle '*hard constraints*' such valve saturation, which are commonly encountered in process plants. Some examples of NMPC applications to bioprocesses are reported in (Hodge and Karim 2002, Parker and Doyle III 2001, Battista, Pico and Marco 2006, Foss, Johansen and Sorensen 1995). Additionally, many of the works in the model-based controllers that are relying on *mechanistic models* are based on the conventional single-scale (or macro-scale) modelling approach.

2.2.7.4 *Model-based Control of Fermentation - Application of Multiscale Models*

Much less works have been reported so far on the attempts to use multi-scale model in the model-based control of fermentation. Nonetheless, an example is reported in the work of (Soni and Parker 2004). In this case, the micro-scale system dynamic is ignored i.e. considered as pseudo-steady state. In perspective, multi-scale NMPC could be one of the next popular extensions of NMPC particularly in bioprocess application because of its inherent capability to handle the multi-scale dynamics. But this might be limited by the progress in the multi-scale modelling and computation.

Discussions on some of the important multi-scale aspects in model predictive control can be found in (Stephanopoulos, Karsligil and Dyer 2000). It is important to note that, one of the major limitations of NMPC is the heavy computational requirement, which so far has currently limited its real-time applications. An excellent review on the currently available computationally efficient NMPC strategies is given by (Cannon 2004).

2.2.7.5 *Model-based Control of fermentation – Application of Non-Mechanistic Models*

Many of the model-based strategies adopted in bioprocesses rely also on the *non-mechanistic* models such as fuzzy system, neural network and hybrid model systems. The advantage of fuzzy system is its ability to model the *complex switches/ nonlinearity*

usually occurring in the microbial systems e.g. physiological switch from the fermentation to *respiro-fermentation* in aerobic yeast cultivation.

In this respect, comprehensive reviews on the use of fuzzy control in bioprocess are reported in (Honda and Kobayashi 2000, Hitzmann, Lubbert and Schugerl 2004, Horiuchi 2002), and industrial-scale applications to bioprocess, e.g. recombinant B₂ vitamin production (Horiuchi and Hiraga 1999) and glutamic acid fermentation (Kishimoto, et al. 1991).

Besides fuzzy models, the neural network models are also adopted in the model-based control of fermentation, for examples, (Chtourou, et al. 1993, Gadkar, Mehra and Gomes 2005, Nagy 2007). The key advantage of neural network model is that its development requires much less process knowledge than what is required for developing mechanistic models. This is very important because, many mechanisms governing the behaviours of microbes are still not known, thus preventing the development of accurate mechanistic models i.e. it is very difficult to develop rigorous mechanistic models for bioprocesses (Aoyama and Venkatasubramanian 1995).

2.2.8 Integrated Bioprocess System – Challenges to Process Control

Today, biotechnological processes have been adopted in almost every aspects of live to produce for examples, biofuels, fine chemicals, medicines, foods and beverages and to treat waste products such as wastewaters and solid wastes from industries. Among these biotechnological products, biofuels production via fermentation has been recognized as the key driver to sustain the industrial civilization in the face of depleting fossil-based fuels resources (Ragauskas, et al. 2006). Other examples include the concept of microbial fuel cell to simultaneously produce electricity or energy and treat wastewater (Rozendal, et al. 2008, Du, Li and Gu 2007), mixed culture biotechnology to simultaneously generate biogases or desired chemicals and to treat wastewater (Kleerebezem and Loosdrecht 2007) and integrated advanced oxidation with biological process (Bankian and Mehrvar 2004).

The increasing trend of integration in bioprocess systems can lead to several challenges to process control design and operation because this integration leads to larger number of possible measurements and operating objectives. A good control

system must be able to meet the operating objectives within a realistic range of operating conditions. It is interesting to note that, the performance of a control system is determined more by the control structure (choice of controlled variables and manipulated variables) rather than the controller algorithms design (Arbel, Rinard and Shinnar 1996). Thus, for the process control to serve as a way to improve bioprocess performance (i.e. process system engineering approach), then the focus should lie in the control structure design aspect and less in the controller algorithm design. Unfortunately, to date, the research works dedicated into the control structure design aspect is far less than that dedicated into controller algorithm design. And yet the integration in bioprocess will inevitably create a challenge to control structure design because it results in a large number of measurements or variables available. Hence, it becomes less clear which output variables to be controlled and which inputs to be manipulated – this issue goes beyond the current consideration of controller algorithm design.

2.3 Bioethanol Production - Overview

The current surge in global oil demand and climate change imperatives has driven the world to think seriously into the large-scale substitute for the petroleum-based fuels. The 2% of today's transportation fuels derived from biomass and blended with fossil fuels are produced either by the fermentation to ethanol of food-derived carbohydrates (such as sugarcane or cornstarch) or by the processing of plant oils to produce biodiesel. Evidently, credible studies show that with plausible technology developments, biofuels could supply some 30% of global demand in an environmentally responsible manner without affecting food production (Koonin 2006). Moreover from the sustainable development perspective, shifting the society's dependence away from petroleum to renewable biomass resources is considered as an important contributor to the development of a sustainable industrial society and effective management of greenhouse gas emissions (Ragauskas, et al. 2006).

Among these diversified biofuels, bioethanol is the most widely used today as a fuel alternative where it constitutes 99% of all biofuels in the United States, which is equivalent to 3.4 billion gallons of ethanol blended into gasoline in 2004 (Davis and Diegel 2004). Interestingly, the most recent studies show that the current technologies of

producing bioethanol from corn are much less petroleum-intensive than gasoline but have greenhouse gas emissions similar to those of gasoline (Farrell, et al. 2006). Even so, it has been widely accepted that bioethanol can only become large substitutes to petroleum-based fuels only if its production becomes economically competitive.

The key challenges for the successful bioethanol industry, as a fuel alternative would hinge in the efficient integration of knowledge across disciplines covering the scientific areas such as plant genetics, biochemistry, biomass chemistry and process engineering. Unlike simple chemical processes, successful process engineering of complex bioprocesses in general would require engineers to properly address the critical issues particularly in the aspects of modelling, design and choice of control strategies. Despite the awareness of the complexity of bioprocesses which normally consist of intermediates reactions pathways catalyzed by numerous of enzymes (Brass, Hoeks and Rohner 1997), the modelling approach for design and control of such systems still largely relies on the macro-scale concept. Bearing in mind the bioprocesses complexity, it is doubtful whether the design and control based on such models would be sufficiently reliable as a basis for real time implementation.

2.4 Extractive Alcoholic Fermentation

It has been well accepted that the conventional alcoholic fermentation technique is a typical product inhibitory processes where the accumulation of ethanol concentration above ca. 12 %(v/v) would drastically reduce the cell growth and ethanol production rates (Minier and Goma 1982). As a result, the conventional alcoholic fermentation exhibits low ethanol productivity and yield that generally restricts its economic competitiveness for the large-scale production. Therefore, low productivity and yield of conventional fermentation has motivated the development of new fermentation technology, which basically relies on the concept of simultaneous fermentation and product removal, for example, the extractive alcoholic fermentation technique.

Earlier works reported on the extractive fermentations (Ramalingham and Finn 1977, Cysewski and Wilke 1977) clearly showed the improvement of its productivity over the conventional technique. Furthermore with cell recycle in extractive fermentation, Cysewski and Wilke (1977) reported that the ethanol productivity could be

further increased by approximately twice as that without cell recycle. Following these earlier discoveries, much of the recent studies have combined the concepts of extractive fermentation and cell recycle in bioreactor as a unified means to effectively achieve high ethanol yield and productivity.

Within the broad family of extractive fermentation, it can be further classified according to approaches of achieving simultaneous fermentation and product removal. Some examples are the fermentation under vacuum (Cysewski and Wilke 1977, Ramalingham and Finn 1977), fermentation combined with flash vessel (Maiorella, Blanch and Wilke 1984, Ishida and Shimizu 1996, Silva, Rodrigues and Maugeri 1999), pervaporation (Christen, Minier and Renon 1990, Shabtai 1991), solvent extraction (Minier and Goma 1982, Barros, Cabral and Novais 1987, Gyamerah and Glover 1996), gas membrane extraction (Gostoli and Bandini 1995), membrane distillation (Calibo, Matsumura and Kataoka 1989, Banat and Simandl 1999) and adsorption (Einicke, Glaser and Schollner 1991).

Also, some works have been reported on the coupling of fermentation with membrane dialysis as a method of relieving product inhibitions (Kyung and Gerhardt 1984). Thibault et al (1987) investigated the possibility of using supercritical CO₂ for *in situ* recovery of ethanol during its production by yeast *S. cerevisiae*. Although it is possible to produce ethanol by fermentation at high pressure (7 MPa), severe inhibition occurred with CO₂ as headspace gas leading to 17% lower ethanol concentration than that under normal fermentation conditions. In contrast, a promising result was reported by employing CO₂ as a stripping agent for ethanol recovery in a bubble column packed with coconut shell charcoal (Pham, Larsson and Enfors 1998). This technique differs from that of Thibault et al (1987) mainly because of the much lower CO₂ pressure was used in the bubble column by the former technique.

Rigorous mathematical model of extractive alcoholic fermentation adopting liquid-liquid extraction can be found from (Fournier 1986). Based on the model, it was shown that the specific productivity can be increased significantly in addition to the ability to ferment a feed with a concentration of sugar, which is several times that is possible in conventional fermentations. From economic point of view, Honda et al. (1987) developed a general framework for assessing the improvement of extractive

fermentation with liquid-liquid extraction as compared with the conventional fermentation.

Although the use of solvent in extractive fermentation could provide both kinetic and thermodynamic advantages, a great deal of effort is required to choose suitable solvent that is completely biocompatible (Bruce and Daugulis 1991). As far as the solvent toxicity is concerned, some work has been reported on how to reduce the toxicities, for examples, the separation of solvent from cell containing broth via membrane perstraction (Frank and Sirkar 1985, Matsumura and Markl 1986, Jeon and Lee 1989), yeast immobilization (Bar 1986) and soybean addition to fermenting broth (Yabannavar and Wang 1991).

The application of membrane pervaporation has the advantages over the other removal techniques, such as process simplicity, less toxicity to fermenting organisms, and less distillation energy consumption. However, some major limitations that hinder its application in large-scale operation is the requirement of low temperature condensation of permeate vapour (O'Brien, Roth and McAlloon 2000), development of a highly ethanol-selective membrane (Calibo, Matsumura and Kataoka 1989) and low permeate flux (Banat and Simandl 1999). On the other hand, Silva et al (1999) reported some of the positive features of extractive fermentation coupled with flash vessel such as (1) ease of operation, (2) low cost, (3) elimination of heat exchanger requirement, (4) low inhibitory conditions for yeast cells, and (5) high inhibitory conditions for contaminants.

2.5 Summary

Research efforts to improve bioprocess performance can be divided broadly into (1) process system engineering, and (2) metabolic engineering approaches. From process system engineering perspective, the applications of process control techniques has received a widespread research attention in the area of bioprocess control. Vast majority of bioprocess control works reported in the past 30 years are related to the controller algorithms design e.g. nonlinear controller design and adaptive controller design. Although control structure (i.e. which variable to control and which variable to manipulate) has larger impact than the controller algorithm design on the overall control

system performance, very little work has been embarked on the former as compared on the latter.

Increasing trend of integration in bioprocess in response to greater challenge to achieve higher profit, more efficient use of raw material and less waste generation has motivated the development of more complex system with large number of variables. As a consequence, the task to determine the proper control structure has become an even more formidable challenge to engineers. This in turn has created large research gaps which must be addressed to improve bioprocess performance via the applications of process control techniques. It is thus no longer sufficient to rely on controller algorithm only – more intensive research in bio-control structure design is required.

Methods to address control structure problems can be divided into 2 main categories: (1) mathematical-based and (2) heuristic-hierarchical approaches. The *data-oriented approach* advocated in this thesis is an emerging method to solve this problem.

Partial control concept provides an attractive solution to control structure problem. However, its main limitation arises from its heavy reliance on process knowledge and experience. Therefore, to exploit the potential of partial control, a systematic tool must be developed which can reduce the heavy reliance on process experience and knowledge.

Fuel ethanol is currently the largest component in biofuels. Because ethanol fermentation is a typical inhibitory process, the ethanol produced during fermentation should be partially removed to reduce its inhibition effects on growth and product formation rates. The extractive alcoholic fermentation technique provides a practical solution to overcome this inhibition problem for ethanolic fermentation process.

3 PARTIAL CONTROL THEORETICAL FRAMEWORK

3.1 Introduction

The concept of Partial Control Structure (PCS) in Chapter 2 could be adopted as a formal framework, within which the control structure problems could be addressed in a systematic manner. But the generalized concept of partial control and its current method of implementation have three limitations: (1) no formal definition for dominant variables, (2) heavy reliance on process experience and knowledge, and (3) lack of clear expression of relationship between performance measures and dominant variables.

In this chapter, we propose a new theoretical framework for partial control within which the definition of *dominant variable* can be clearly stated. Furthermore, the development of this new framework is crucial because it leads to the development of a novel procedure to identify the dominant variables known as the *PCA-based technique*.

3.2 General Concept of Partial Control

Kothare et al. (2000) developed a framework for partial control. Here, this framework is adopted with some modifications. Suppose the plant to be controlled is described as:

$$\dot{\chi}(t) = F(\chi(t), U(t)) \quad 3-1$$

Note that, this representation is slightly different from that of Kothare et al. (2000) where they explicitly divided the input variables as manipulated and disturbance variables. In this case, we simply lump both types of inputs as represented by vector $U \in R^{n_u}$ i.e. $U = [U_{mv} \ D]^T$ where U_{mv} is a vector of manipulated variables and D is a vector of disturbance variables. Meanwhile, $\chi \in R^{n_x}$ is the vector of system states and F is generally a nonlinear function of its arguments. The vector of output variables $Y \in R^{n_y}$ can be expressed as:

$$Y(t) = G(\chi(t), U(t)) \quad 3-2$$

Let the vector of measured outputs $Y_p \in R^{n_p}$ be a vector of process variables (excluding input variables), which define the process specifications (i.e. set of operating objectives) where $Y_p \subseteq Y$ i.e. $n_p \leq n_y$. Here, Y_p can be expressed as a nonlinear relationship as:

$$Y_p(t) = G_p(\chi(t), U(t)) \quad 3-3$$

Because Y_p defines the control objectives (e.g. stability, product specifications, etc), it is important to control Y_p at the setpoint Y_p^{ss} . Now, depending on the number of manipulated variables available (i.e. size of U_{mv}), one can adopt either *exact control* or *partial control*. According to Kothare et al. (2000) exact control can be defined as:

Definition 3.1: Exact Control

The system described by Eq. 3-1 and Eq. 3-2, without any constraints on U_{mv} is said to be exactly controllable if Y_p (vector of performance variables) can be moved to and maintained at an arbitrary prescribed set point Y_p^{ss} without offset, starting from an arbitrary initial point, by an appropriate (possibly) nonunique choice of the steady-state value of manipulated variable.

□

In practice, most process plants possess far less number of manipulated variables than the number of measured outputs – i.e. *thin* plant. So, it is not possible to apply exact control strategy to such processes. Thus in this case, partial control is the only option where it can be defined as:

Definition 3.2: Partial Control

The system described by Eq. 3-1 and Eq. 3-2, without any constraints on U_{mv} is said to be partially controllable if the vector of performance variable Y_p can be moved to and maintained within an acceptable range of an arbitrarily prescribed set point Y_p^{ss} , starting from an arbitrary initial point and by an appropriate (possibly non-unique) choice of the steady-state value of manipulated variable U_{mv} , such that to ensure $Y_{p,min}^{ss} \leq Y_p \leq Y_{p,max}^{ss}$ in the face of external disturbances occurrence.

□

3.3 Partial Control Problem Formulation: New Framework

Note that, the general representation previously described as Eq. 3-3 cannot clearly reveal the essence of the partial control problem, especially when the performance objective is an *implicit function* of the input-output variables. It is not clear from this representation whether all of the elements in Y_p are the dominant variables or only some of the elements in Y_p are dominant variables. Nor it is obvious how Y_p is related to the performance measures.

Thus, we propose a more direct representation of a performance measure ϕ_p as follows:

$$\phi_p = F_p(U, Y, B) \quad 3-4$$

Here, $B \in R^{n_\beta}$ is a vector of process parameters and F_p is a function of its arguments. The performance measure represented by Eq. 3-4 can be directly one of the elements in the measured output set Y_p (i.e. $\phi_p = y_p$ where $y_p \in Y_p$). Additionally, ϕ_p can be an implicit function of the process variables and parameters such as, optimum profit or minimum cost of production.

From Eq. 3-4, we can further express the performance measure explicitly in terms of the dominant and minor variables as:

$$\phi_p = F_p(U_{D,p}, Y_{D,p}, B_{D,p}, U_{M,p}, Y_{M,p}, B_{M,p}) \quad 3-5$$

Here, $U_{D,p}$, $Y_{D,p}$ and $B_{D,p}$ correspond to the sets of inputs, outputs and parameters, which have the dominant effects on ϕ_p and thus, they are referred to as the *dominant variables*. Meanwhile $U_{M,p}$, $Y_{M,p}$ and $B_{M,p}$ are sets of inputs, outputs and parameters, which only have minor or small contributions to ϕ_p and referred to as the *minor variables*.

Now, let $\Omega_p = \{U_{D,p}, Y_{D,p}, B_{D,p}\}$ and $\Psi_p = \{U_{M,p}, Y_{M,p}, B_{M,p}\}$ are the sets of variables corresponding to dominant and minor variables respectively. Furthermore, assuming that the contributions of the dominant and minor variables to the performance measure ϕ_p can be *linearly* combined (i.e. over the specified range of operating conditions), so that, it can be written as:

$$\phi_p = F_{D,p}(\Omega_p) + F_{M,p}(\Psi_p) \quad 3-6$$

Where $F_{D,p}$ and $F_{M,p}$ are functions that represent the *contributions* of the dominant and minor variables sets respectively to the performance measure ϕ_p where $p = 1, 2, 3 \dots n$.

Remark 3.1:

The Eq. 3-6 assumes that the dominant and minor variables have no interacted term i.e. contributions by both sets of variables can be combined linearly. It is important to note that, $F_{D,p}$ and $F_{M,p}$ could be either linear or nonlinear functions of their arguments. Normally these functions are unknown; otherwise we can directly identify the dominant variables from Eq. 3-6. If the functions are known, then we still need to define the range of operating conditions over which they are valid. This is important because we expect that dominant and minor variables sets can vary over a large operating conditions due to the process nonlinearity i.e. a dominant variable at one operating level can become a minor variable at another, or vice versa. However, the representation of the dominant and minor variables contributions to ϕ_p as Eq. 3-6 is necessary in order to proceed with the formal definition of the dominant variables. Only after making clear definition of the dominant variables can we then proceed to develop the PCA-based technique to identify the dominant variables.

□

Following Eq. 3-6, a general partial control problem can now be stated as follows:

(P-3.1)

Given a set of variables (including process parameters) and a performance measure ϕ_p (Eq.3-6), identify the set of dominant variables (Ω_p) that corresponds to the given performance measure.

□

This general problem **(P-3.1)** can be illustrated by Figure 3-1, which shows the *mapping* of a set of dominant variables onto a performance measure ϕ_p and where the set of all variables making up the process plant is $\Sigma = \{U, Y, B\}$, where $\Omega_p \subset \Sigma$. This is a very difficult problem to solve if the method used to identify the dominant variables solely relies on engineering experience and process knowledge. As the sizes of Σ and

Φ are getting larger, the more complicated the problem becomes, which in turn can easily lead to unreliable result.

Remark 3.2:

From Figure 3-1, $\Omega_2 \cap \Omega_3 \neq 0$ thus, ϕ_2 and ϕ_3 are said to be correlated with each other. On the other hand $\Omega_1 \cap \Omega_2 = 0$ thus, ϕ_1 and ϕ_2 are said to be uncorrelated with each other. The complete dominant variable set Ω_T for n number of performance objectives is a combination of all these dominant variable sets i.e. $\Omega_T = \Omega_1 \cup \Omega_2 \cup \Omega_3 \dots \Omega_n$.

□

From the control performance point of view, one is probably more interested in knowing how much the performance measures will vary when external disturbance occurs. Such a variation in the performance measure ϕ_p from its steady-state nominal value may be written as:

$$\Delta\phi_p = \Delta F_{D,p} + \Delta F_{M,p} \quad 3-7$$

Where the contributions (norm values) are given as:

$$\Delta F_{D,p} = \|F_{D,p}(\Omega_p) - F_{D,p}(\Omega_p^{ss})\| \quad 3-8$$

$$\Delta F_{M,p} = \|F_{M,p}(\Psi_p) - F_{M,p}(\Psi_p^{ss})\| \quad 3-9$$

Note that, Ω_p^{ss} and Ψ_p^{ss} correspond to the steady-state (nominal) values of dominant and minor variables sets respectively. For n number of performance measures (i.e. multiple objectives), a vector of variations can be written as:

$$\Delta\Phi = \begin{bmatrix} \Delta\phi_1 \\ \Delta\phi_2 \\ \vdots \\ \Delta\phi_n \end{bmatrix} = \begin{bmatrix} \Delta F_{D,1} \\ \Delta F_{D,2} \\ \vdots \\ \Delta F_{D,n} \end{bmatrix} + \begin{bmatrix} \Delta F_{M,1} \\ \Delta F_{M,2} \\ \vdots \\ \Delta F_{M,n} \end{bmatrix} \quad 3-10$$

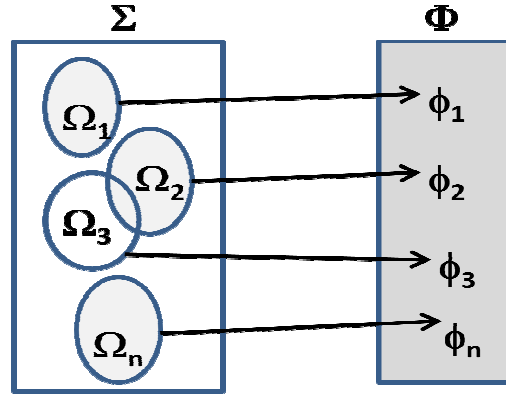


Figure 3-1: Illustration of the key problem of partial control: mapping of set of dominant variables onto performance measures

3.3.1 Dominant Variable Definition

Based on Eq. 3-7 or Eq. 3-10, we can now proceed with the definition of the dominant variable with respect to a given performance measure as follows:

Definition 3.3: Dominant Variable

The dominant variables set Ω_p for a given performance measure ϕ_p is defined as the smallest subset of variables that can (possibly) be formed from the set $\Sigma = \{U, Y, B\}$ such that, when the variables in Ω_p are controlled at constant values (or setpoints), the variations in dominant variables $\Delta F_{D,p} = 0$, and as such the variation in performance measure is solely due to the variations in minor variables (i.e. $\Delta F_{M,p} \neq 0$) and such that $\Delta \phi_p = \Delta F_{M,p} \leq \Delta \phi_{p,max}$.

□

Remark 3.3:

The Definition 3.3 above implicitly assumes that there is no interaction among the dominant variables. Thus, we assume that they are all selected as controlled variables which mean that their variations from their nominal values are zero. It is interesting to point out that in most cases, these dominant variables are interacted among themselves and as such it is not necessary to control all of them in practice. If this is the case, then $\Delta F_{D,p} \neq 0$ but we still expect that $\Delta \phi_p \leq \Delta \phi_{p,max}$ if the variables that are being controlled are indeed the dominant variables. In this regard, the presence of interaction

among the variables often leads to the identification of only a small subset of the dominant variables if the methods used for their identification relies on process experience or optimization. Therefore, Definition 3.3 above consider the entire set of dominant variables rather than only this small subset i.e. if $\Delta F_{D,p} \neq 0$.

□

3.3.2 Mathematical Formulation of Partial Control

Following the Definition 3.3, the variable in the set Ω_p is the dominant variable corresponding to the performance measure ϕ_p . In other words, this variable is bound to have strong influence on the performance measure ϕ_p but not necessarily on the other performance measures.

An alternative problem statement based on the optimization framework can also be derived from the definition of partial control (Definition 3.2) and the general representation of Eq. 3-10 (i.e. in term of norm of variations of performance measures).

The “simplest” mathematical representation for the partial control problem can be viewed as an optimization problem as follows:

(P-3.2)

$$\min_{\Omega_{CS} \in \Sigma} (\Delta \Phi(U, Y, B))$$

Subject to:

$$N_{CS} \leq N_{U_{mv}} \tag{3-11}$$

$$\Delta \Phi \leq \Delta \Phi_{max} \tag{3-12}$$

$$U_{min} \leq U_{mv} \leq U_{max} \tag{3-13}$$

$$D_{min} \leq D \leq D_{max} \tag{3-14}$$

$$G(U, Y, B) = 0 \tag{3-15}$$

Note that, the variations of the performance measures $\Delta \Phi$ from their nominal values in the presence of external disturbances are measured in term of Euclidian norm. The notation N_{CS} stands for the total number of dominant variables in Ω_{CS} . Here, Ω_{CS} denotes the total set (i.e. $\Omega_{CS} = \Omega_1 \cup \Omega_2 \cup \dots \cup \Omega_n$) of the dominant variables

corresponding to a set of performance measures ϕ_p , which are assumed to be controlled at the constant setpoints. And $N_{U_{mv}}$ is the total number of available manipulated variables (or control degree of freedom). Meanwhile, the manipulated variables are assumed to be constrained between the maximum and minimum values of U_{max} and U_{min} respectively. Moreover, the optimization is subject to an anticipated vector of disturbances D with lower and upper bounds equal to D_{min} and D_{max} , respectively.

It is important to note that, this is contrary to the definition of partial control (Definition 3.2) where the manipulated variables are not constrained. However, if such constraint on manipulated variables is not imposed, then the optimization result can be infeasible for the specified range of operating conditions or *window*. The reason for this is that different operating window can lead to different dominant variables for similar performance objectives – for nonlinear system the control structure depends on operating level (Nandong, Samyudia and Tade 2007b). Meanwhile, G represents a set of equations which describes the steady-state behaviour of the process. Note that, the dynamic model is required if the set of performance measures contains a dynamic performance measure.

Bear in mind that, the representation of partial control problem **P-3.2** implicitly assumes that all of the dominant variables must be selected as controlled variables. In practice, the problem as stated by **P-3.2** can be extremely difficult to solve by means of conventional mathematical method. The presence of multiple performance measures can significantly complicate the identification of dominant variables due to the *interrelated* natures of the variables. Moreover, such optimization problem normally requires large computational time due to the combinatorial nature of the problem and nonlinearity. However, this representation is useful because it can help us to view the *essential feature* of the problem in its simplest form possible.

Additionally, depending on which approach is employed to find the dominant variables, either by heuristic (**P-3.1**) or by mathematical (**P-3.2**), it is quite unlikely that the resulting dominant variables obtained by both approaches will be exactly the same i.e. $\Omega_T \neq \Omega_{CS}$. Recall that, the Ω_T represents the set of total dominant variables

corresponding to all performance objectives obtained by heuristic approach (**P-3.1**) and Ω_{CS} represent the total set of dominant variables obtained by solving **P-3.2**.

Consequently, this means that the technique for identifying the dominant variables can become a decisive factor that determines the performance of partial control strategy. One reason for this is that partial control performance is heavily dependent on the selection of controlled variables, which necessarily come from the set of dominant variables identified.

3.4 Basic Concepts for PCA-based Technique

3.4.1 Principal Component Analysis (PCA)

For more details about the PCA, interested readers could refer to Wise and Gallagher (1996). Here we just provide brief overview about PCA and its property which is relevant to the proposed technique. Assuming that the data matrix X has m rows (observations) and n columns (variables plus performance measures), the application of PCA to the dataset will decompose X into the sum of outer product of vectors t_i and p_i plus a residual matrix E :

$$X = t_1 p_1^T + t_2 p_2^T + \cdots + t_k p_k^T + E \quad 3-16$$

Where $k \leq \min(m, n)$, the vector t_i is known as scores and the vector p_i is called loadings. While the scores provide the information on how the samples or observations relate to each other, the loadings contain the information on how variables are interrelated.

Remark 3.4:

The matrix of dataset X should contain both variables and performance measures of interest. Thus, the number of columns consists of the number of variables (n_v) and performance measures (n_ϕ) i.e. $n = n_v + n_\phi$.

□

To determine which variables are responsible for certain *abnormal event*, one can plot the scores and loadings of the first and second principal components (PC-1 and PC-2) as depicted by Figure 3-2. From this PCA plot one can then identify the *outlier* or the

observation point that is far away from the centre i.e. outside the normal *operating window* (shown by dotted circle). This outlier is normally related to the *unusual* or *abnormal* event that occurs in the system. The variables which occupy the same quadrant as the outlier (i.e. 1st quadrant) and the opposite quadrant (i.e. 3rd quadrant) are expected to have some influences on the occurrence of the outlier (see Figure 3-2).

Moreover, the variables that occupy the same quadrant as the outlier are *positively* correlated with the outlier and those occupying the opposite quadrant are *negatively* correlated with the outlier. Likewise, the variables in the same quadrants are positively correlated with each other but negatively correlated with those in the opposite quadrant.

If the variables are positively correlated with the outlier, then this means that in order to reduce the outlier one needs to reduce the values of the variables, and vice versa. *The question now becomes how can one use this concept to identify the dominant variables?*

Suppose that an outlier exists and based on the PCA plot, one can identify a variable and a performance measure which are strongly responsible for this outlier. Then, one can conclude that the variable must have a very strong influence in comparison with other variables on the performance measure. Thus, we say that this variable is a dominant variable for the performance measure. However, for this analysis to work we need to develop a proper procedure involving the use of not only PCA but also design of experiment (DOE) concept. Furthermore, we need to establish certain criteria and conditions to be used together with the procedure.

3.4.2 Dominant Variable Identification

3.4.2.1 Conceptual Framework for PCA-Based Technique

Figure 3-3 illustrates the PCA-based technique which involves successive applications of PCA on a dataset X , i.e. successive dataset reductions are required. The first application of PCA (i.e. 1st level of dataset reduction) on the original dataset X (Figure 3-3a) generates two uncorrelated sub-groups (orthogonal groups) of smaller sub-datasets X_1 and X_2 :

$$X = [X_1 \quad X_2]$$

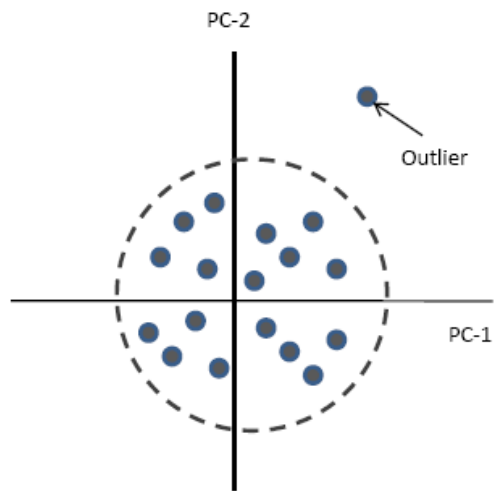


Figure 3-2: Plot of scores and loadings of PC-1 and PC-2

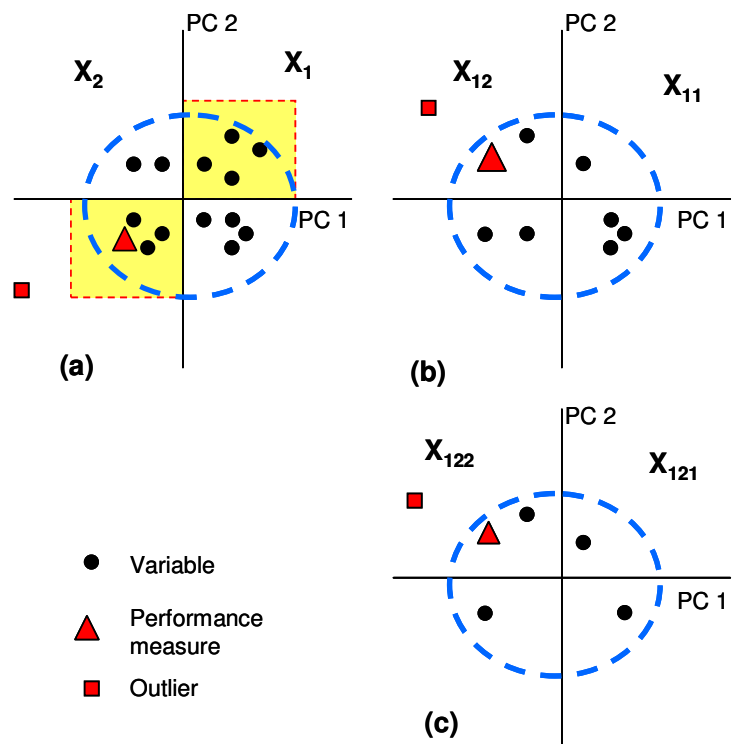


Figure 3-3: Generalized concept of dataset reduction using PCA to identify dominant variables

Here, the subscript “1” is to indicate the subset of variables and performance measures that occupy the 1st and 3rd quadrants. And the subscript “2” is to indicate those variables and performance measures that occupy the 2nd and 4th quadrants. Also note that, X_1 and X_2 are called the first level of reduced sub-datasets.

From Figure 3-3a, the sub-dataset X_1 contains the performance measure of interest. But at the level of this dataset reduction, it remains unclear which of the variables (out of the 7) that strongly *correlate* with the performance measure i.e. its dominant variables.

Therefore, another PCA is applied to the sub-dataset X_1 as shown in Figure 3-3b and this generates even smaller two sub-datasets as:

$$X_1 = [X_{11} \quad X_{12}] \quad 3-18$$

Note that, this is called second (2nd) level of dataset reduction where the *last* number in the subscript indicates which quadrants the sub-dataset belongs to e.g. X_{12} , where number “2” indicates that the sub-dataset belongs to quadrants 2 and 4 and number “1” indicates the previous “parent” sub-dataset.

Now from Figure 3-3b, one can see that the performance measure of interest is in the X_{12} . As expected, the number of variables has now been reduced from 7 to 4 variables. Another PCA can be applied to X_{12} and further reduces this sub-dataset as:

$$X_{12} = [X_{121} \quad X_{122}] \quad 3-19$$

Finally, from Figure 3-3c, one can identify that the performance measure is now in the 3rd level of sub-dataset X_{122} and there are only two variables that are deemed having *strong* correlation with the performance measure. And these two variables are most likely the dominant variables for the performance measure.

Remark 3.5:

It is important to note that, the PCA plot (Fig. 3-3) based on which a dataset is successively reduced is only involved the first two principal components i.e. PC-1 and PC-2. The plot of PC-1 and PC-2 is considered adequate if the sum of variances of PC-1 and PC-2 is at least 70% of the total variances in the original dataset. Of course, this

sum of variances of PC-1 and PC-2 normally increases with the increase in the level of dataset reduction.

□

3.4.2.2 Dominant Variable (DV) Criteria

There are 3 conditions that constitute the so-called *dominant variable (DV) criteria*, which states that for the dataset or sub-dataset to contain any dominant variable:

- 1) There should be at least one performance measure in the dataset.
- 2) There should be at least one variable in the dataset.
- 3) There should be at least one outlier exists within the dataset.

If one or more of these criteria are not fulfilled, then the set of variables obtained cannot be guaranteed as the dominant variables set.

3.4.2.3 Successive Dataset Reduction (SDR) Condition

If the dominant variables are identified through successive dataset reductions, then the *successive dataset reduction (SDR) condition* must be fulfilled, which states as follows:

For the successive dataset reductions using PCA, at each level of dataset reduction the DV criteria must be completely fulfilled, else the dominant variable identification result is not consistent.

Therefore, based on the previous illustrative example (Figure3-3), notice that the 3 criteria are fulfilled throughout the 3 stages in the dataset reductions. Thus, the dominant variable identification result is consistent.

3.4.2.4 Critical Dominant Variable (CDV) Condition

In connection to the successive dataset reduction process, an important question is how many successive dataset reductions are required before one can “safely” conclude that the dominant variables have finally been revealed. In response to this question, we introduce a *stopping* condition, which is termed as the *critical dominant variable (CDV) condition*.

Definition 3.4: Critical Dominant Variable Condition

The successive dataset reduction level is said to reach a critical dominant variable condition once the sum of variances of principal components associated with the dataset reduction level, which are used to generate the PCA plot $\geq v_{cric}$.

□

Notice that, as the successive dataset reduction level increases, the sum of variances of principal components used to generate the PCA plot also increases. The successive dataset reduction can be stopped once this sum of variances reaches the threshold value (v_{cric}). Normally, we prefer a 2D-plot of PCA, which requires only the first two principal components (PC-1 and PC-2) as shown previously in the illustrative example (Figure 3-3). Once the sum of variances of PC-1 and PC-2 has reached a value that is at least equal to v_{cric} then, this implies that the dominant variables have already been identified at the corresponding dataset reduction level i.e. the critical level of dataset reduction level has been achieved.

If the sum of variances of PC-1 and PC-2 (i.e. 2D-plot of PCA) is not large enough, the result obtained may not be accurate. Thus, one may need to plot PC-1, PC-2 and PC-3 (i.e. 3D-plot). Here, the sum of variances of the PC-1, PC-2 and PC-3 must be at least equal to v_{cric} . Note that, in the case study described in this thesis, we take the value of $v_{cric} = 85\%$.

3.4.3 Concept of Closeness Index

The closeness of variables (including parameters) V_i to Φ_j can be calculated by measuring the distance between V_i^* and Φ_j (see Figure 3-4), where V_i^* is the resolved location of V_i in the direction of the Φ_j . Here, V_i can be a process input u , or output y , or parameter β .

Definition 3.5: Closeness Index

The *closeness index* (CI) which is a measure of the strength of correlation between variable V_i and a performance measure Φ_j in the direction of the performance measure is defined as follows:

$$\delta_{ij} \triangleq \|D_{ij}\|/\|\overrightarrow{O\Phi_j}\| \quad 3-20$$

Where the distance between the resolved position V_i^* and position Φ_j (Figure 3-4) can be written as:

$$D_{ij} = \|\overrightarrow{O\Phi_j}\| - \|\overrightarrow{OV_i^*}\| = \|\overrightarrow{O\Phi_j}\| - \|\overrightarrow{OV_i}\|\cos(\theta) \quad 3-21$$

The value of δ_{ij} provides the measure of how close the correlation between a variable V_i and a performance measure Φ_j . The smaller the magnitude of δ_{ij} then the more closely is the correlation between V_i and Φ_j . Note that, the closeness index can also be calculated between two dominant variables. Let says one wants to find out how close is the correlation of a variable V_k in the direction of another variable V_i .

Then the closeness index can be written as:

$$\delta_{ki} = \|D_{ki}\|/\|\overrightarrow{OV_i}\| \quad 3-22$$

Of course, one can also find out how close is the correlation between V_k and V_i in the direction of V_k . In this case, the closeness index in the direction of V_k is:

$$\delta_{ik} = \|D_{ik}\|/\|\overrightarrow{OV_k}\| \quad 3-23$$

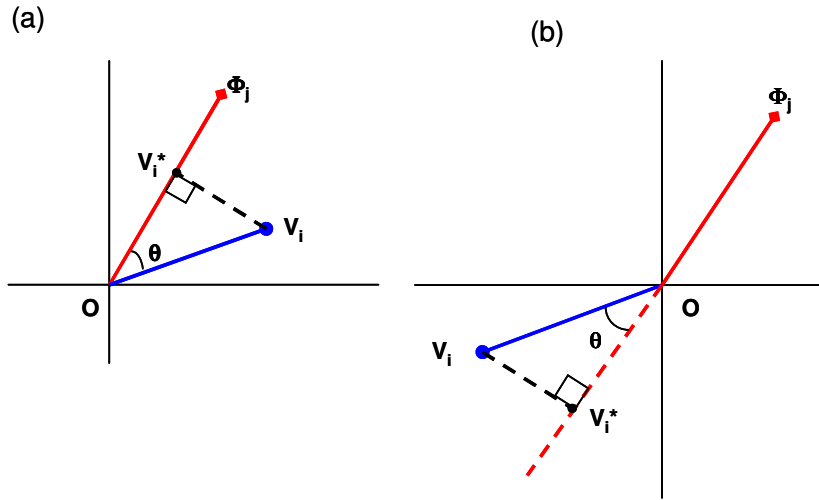


Figure 3-4: Illustration of closeness index concept: (a) V_i is positively correlated with Φ_j , and (b) V_i is negatively correlated with Φ_j

It is important to note that, the value of δ_{ki} is not necessarily the same as δ_{ik} . Therefore, this has an important implication on the selection of controlled variable as will be discussed in the next section. The significances of closeness index can be summarized as following:

1. For a given performance measure ϕ_p and multiple dominant variables y_1, y_2, \dots, y_n , the values of closeness index i.e. $\delta_{1p}, \delta_{2p}, \dots, \delta_{np}$ can provide the order of influences of the variables on the performance measure.
2. For a given dominant variable y_k and a multiple performance measures ($\phi_1, \phi_2, \dots, \phi_p$) which are correlated with y_k , then the values of closeness index i.e. $\delta_{k1}, \delta_{k2}, \dots, \delta_{kp}$ provide the order of influence of y_k on the performance measures.
3. When the set of dominant variables corresponding to a performance measure ϕ_p consists of an input u_m and output y_n , then the values of δ_{mp} and δ_{np} provide the clue whether u_m can be used as manipulated variable for y_n . If $\delta_{mp} < \delta_{np}$ then this suggests that u_m should not be considered as manipulated variable.

4. Let suppose for a given performance measure ϕ_p there exist two dominant variables y_i and y_j that have similar or very comparable closeness index $\delta_{ip} = \delta_{jp}$ then, the calculation of δ_{ij} and δ_{ji} provides the clue whether to control both dominant variables or only one of them. If the values of δ_{ij} and δ_{ji} are small, then it is sufficient to control y_i if $\delta_{ij} < \delta_{ji}$, otherwise control y_j . When the values of δ_{ij} and δ_{ji} are significantly large then, this suggest it is better to control both of the dominant variables i.e. more variables need to be controlled.

Note that, the closeness index (CI) is used to form two types of matrices, called the dominant variable interaction index and variable-variable interaction index. While CI itself can be used for ranking the dominant variables, the two indices can be used for assessing the *sufficient* number of controlled variables (i.e. either primary or inventory or constraint controlled variables) required. Applications of the dominant variable interaction and variable-variable interaction indices will be demonstrated in Chapters 7 and 8.

3.4.4 Ranking of Dominant Variables by Closeness Index

There are two types of rankings:

Case 1: *Multiple Variables – Single Performance Measure (MVSPM) Ranking*

For a given ϕ_p and multiple variables, ranks the strength of influences of y_1, y_2, \dots, y_n on ϕ_p based on the values of $\delta_{1p}, \delta_{2p}, \dots, \delta_{np}$.

Case 2: *Multiple Performance Measures - Single Variable (MPMSV) Ranking*

For a given dominant variable y_i and multiple performance measures correlated with it, ranks the influence of y_i on $\phi_1, \phi_2, \dots, \phi_m$ based on the values of $\delta_{i1}, \delta_{i2}, \dots, \delta_{im}$.

Illustrative Example 1: Case 1

Let a dataset X which contains 6 variables and 2 performance measures as follows:

$$X = [y_1 \quad y_2 \quad y_3 \quad y_4 \quad y_5 \quad y_6 \quad \phi_1 \quad \phi_2]$$

Find the most suitable controlled variable that is strongly related to the performance measure ϕ_1 .

Solution 1

Let assume that the first level of dataset reduction on X generates $X_1 = [y_1 \ y_2 \ y_5 \ \phi_1]$ and $X_2 = [y_3 \ y_4 \ y_6 \ \phi_2]$. Assume that the DV criteria and critical dataset reduction level condition are met, then the dominant variable for ϕ_1 are $\{y_1, y_2, y_5\}$.

Computation of closeness index of each variable in the direction of the performance measure ϕ_1 shows that $\delta_{51} < \delta_{11} < \delta_{21}$. Then, the decreasing order of dominant variable influence on ϕ_1 can be deduced as:

$$\begin{array}{c} y_5 \quad y_1 \quad y_2 \\ \longrightarrow \text{decreasing order} \end{array}$$

Thus, y_5 is the strongest dominant variable for the performance measure ϕ_1 which suggests it is the best choice for the controlled variable. Note that, the closer is the variable y_i to a given performance measure ϕ_j , the stronger is the influence of that dominant variable on the performance measure. Hence, given multiple dominant variables the value of δ_{ij} can be used as a basis to choose which dominant variable to be used as the controlled variable.

□

Illustrative Example 2: Case 2

Suppose a dataset X_{11} containing 1 dominant variable and 3 performance measures as follows:

$$X_{11} = [y_i \ \phi_1 \ \phi_2 \ \phi_3]$$

Rank the influence of the dominant variable on the 3 performance measures.

Solution 2

Let suppose that the calculation of the closeness index of y_i in the direction of each performance measure shows that $\delta_{i2} < \delta_{i1} < \delta_{i3}$. Hence, this suggests that y_i has the largest influence on ϕ_2 and the weakest influence on ϕ_3 . The decreasing order of influence of y_i on the performance measures is:

$$\begin{array}{ccc} \phi_2 & \phi_1 & \phi_3 \\ \longrightarrow & \text{decreasing order} \end{array}$$

□

3.4.5 Dominant Variable Interaction Index (I_{DV})

For the case where there are multiple dominant variables, then one of the important considerations is on the degree of their interaction. It is important to know the influence of a particular variable in the direction of other variables because this will determine how many dominant variables that should be controlled.

A matrix of dominant variable interaction (I_{DV}) with n rows of dominant variables and m columns of performance measures in term of the CI values is written as follows:

$$I_{DV} = \begin{bmatrix} \delta_{11} & \delta_{12} & \cdots & \delta_{1m} \\ \delta_{21} & \delta_{22} & \cdots & \delta_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \delta_{n1} & \delta_{n2} & \cdots & \delta_{nm} \end{bmatrix} \quad 3-24$$

Definition 3.6: Dominant Variable Interaction Index (I_{DV})

The dominant variable interaction index is a matrix consisting of n variables and m performance measures of the CI values as Eq. 3.23, which is a measure of influence of a particular variable on performance measures.

□

The significance of I_{DV} is that it can be used as a guideline to decide on how many dominant variables need to be controlled in order to ensure that the variation in the corresponding performance measure ϕ_k is minimal or acceptable. In general, large values of elements in I_{DV} indicate weak coupling between the variables and the performance measures involved. In other words, we cannot guarantee that the variation in the performance measure is acceptable if only one variable is controlled to constant setpoint because of weak correlation with the performance measure. More details regarding the I_{DV} and its extension to a more general case of variables interaction (i.e. variable-variable interaction index I_{VV}) will be further discussed in Chapter 4.

3.5 Summary

In this chapter, a new theoretical framework of partial control is proposed within which the dominant variable can clearly be defined. Also the performance measures-dominant variables relationship is expressed mathematically, which helps to visualize the key problem in partial control. Within the new framework of partial control, the significance of the dominant variables is attached to the existence of *overall (implicit) performance measures*, which are assumed to be the implicit functions of process variables. In contrast, within the classical or generalized framework of partial control, the significance of the dominant variables is attached to the so-called *performance variables*, which define the complete (i.e. overall, inventory and constraint) control objectives of the plant. As will be pointed out in the next Chapters 4 and 7, this approach leads to complication in determining the suitable controlled variables i.e. leads to *non-uniqueness* of sets of dominant variables.

The conceptual framework for applying the PCA-based technique is developed to identify the dominant variables which correspond to the specified performance measures. It is important to note that early development of this technique was reported in (Nandong, Samyudia and Tade 2007b) – but still without a formal theoretical framework for the application of PCA. This PCA-based technique and the new framework of partial control are fused together to form a methodology for solving the partial control problem in particular, and the control structure problem in general. In this case, the partial control framework is required to provide a sound theoretical foundation for the methodology, so that the control structure problem can be addressed in a systematic manner. More details regarding this methodology will be described in the next chapter.

The concept of Closeness Index (CI) is proposed to rank the importance of dominant variables. Additionally, the dominant variable interaction index is developed from the concept of closeness index, which can be used to assess the sufficient number of dominant variables that should be controlled, thus helping us to answer the question of how many controlled variables are required?

4 METHODOLOGY OF COMPLETE PARTIAL CONTROL DESIGN

4.1 Introduction

Previously in Chapter 3, we have elaborated on how the concept of principal component analysis (PCA) can be applied to identify the dominant variables, which is an essential step in the partial control design. Additionally, the definition of dominant variables is also proposed in Chapter 3 in order to clarify the task of dominant variables identification. New concepts such as the closeness index (CI) and the dominant variable interaction index or array (I_{DV}) are also proposed, which can be used to facilitate the selection of controlled variables among a subset of dominant variables.

The key aim of this chapter is to establish a methodology of the so-called *Complete Partial Control Design (CPCD)*, which is based on the results (i.e. PCA-based technique and the new partial control framework) of theoretical development described in Chapter 3. Here, CPCD means that the incorporation of inventory and constraint control objectives into the design of partial control strategy.

4.2 Classification of Control Objectives

In this thesis, it is assumed that the plantwide control objectives can be broadly divided into 3 major categories:

- a) Overall operating objectives/ performance measures.
- b) Inventory control objectives.
- c) Constraint control objectives.

The essential feature of the overall operating objectives is that they are normally *implicit* function of the process variables. For instances, the optimum profit, minimum cost and optimal tradeoff between yield and productivity – thus, they cannot be directly identified from process knowledge or experience. Normally it is very difficult to identify variables which are strongly linked (and hence to be controlled) to these type of control

objectives by means of process knowledge and experience; which variables to be controlled such that the overall performance measures can be achieved. Indeed, the *heart* of the CSD problem is how to address this issue in a systematic way.

It is important to note that for a given set of overall performance objectives, the corresponding set of dominant variables depends on the process design and operating level. Thus, this prevents direct extension of the engineering experience from one process design to another as the dominant variables depend on how the various units comprising the plant are linked together. Furthermore, due to process nonlinearity the dominant variables corresponding to a given set of overall performance objectives can change as the operating level (or condition) changes. Hence, for these two reasons we need a systematic procedure to address a given set of overall performance objectives because it cannot be solved simply by applying process knowledge and experience.

Unlike the overall performance objectives, the inventory and constraint control objectives can directly be handled via our process (or unit operation knowledge) and experience. The significances of inventory control objectives can be summarized as follows:

- a) To prevent overflow or dry up of tanks, reactors, etc. containing liquid.
- b) To minimize the fluctuation of liquid holdup especially in reactor, otherwise this can cause high fluctuation in reactor conversion. Also, small variation in reactor holdup is desirable because it allows the operation closed to the maximum reactor volume, which normally leads to economic advantage.
- c) To prevent material accumulation in the system.
- d) To ensure stability especially if the system is non self-regulating.

The overall aim of the constraint control objective is to ensure that the plant can run in a *safe*, *smooth* and *reliable* manner. To achieve this overall aim, it is important to control the variables which relate to the process constraints, which can be categorized into 4 key areas as:

- i. Safety
- ii. Smooth operation
- iii. Environmental protection
- iv. Product quality

Safety

This includes the safety of both personnel and equipment in the plant. For examples, maximum pressure in distillation column above which the column ruptures, maximum hotspot temperature in exothermic tubular catalytic reactor beyond which runaway reaction occurs, and maximum furnace temperature above which the tubes start to melt.

Note that, the violation of these constraints can cause damage to the equipment involved or severe accidents to the personnel and other equipment in the plant. While the constraints above are typical in process plant, in bioprocess plant one needs to consider even wider scope of constraints, which can strongly affect the productivity and yield. For instance, excessively high temperature can cause irreversible damage to the living cells causing poor productivity or even a complete halt in operation.

Smooth operation

Some variables are very crucial to the smooth operation of the plant, for instance, vapour velocity in distillation column. Whereas too high vapour velocity can lead to flooding, too low vapour velocity can cause weeping. Both phenomena can severely degrade the purities of distillation products and can ultimately lower the productivity. Therefore, it is very important to ensure that the vapour velocity is within an acceptable range during the distillation operation in order to avoid these phenomena. In this case, because we cannot directly measure and control the vapour velocity, we can control the differential column pressure which relates to the vapour velocity.

Environmental protection

The need to protect the health of environment normally leads to certain environmental regulations, which can impose constraints on the process operation. For examples, discharge limits imposed on certain chemicals in wastewater and maximum allowable wastes disposal to the environment.

Product quality

This is an important type of constraint which arises from the market demand. Examples of variables within this class of constraint are the product purity, crystal size distribution, molecular weight of polymer, colour and texture of certain food products, etc.

4.3 Classification of Controlled Variables

Based on the classification of the 3 operating objectives, there are also 3 corresponding types of controlled variables, which are:

- a) Primary controlled variables $Y_{CV,P}$
- b) Inventory controlled variables $Y_{CV,I}$
- c) Constraint controlled variables $Y_{CV,C}$

The following definitions are applied in this thesis regarding the types of the controlled variables mentioned above.

Definition 4-1: Primary Controlled Variables

The primary controlled variables are the dominant variables which are to be controlled at constant setpoints, such that the variations in the key performance measures or overall operating objectives are within the maximum allowable limits.

□

Definition 4-2: Inventory Controlled Variables

The inventory controlled variables are the variables which must be controlled in order to avoid overflow or dry up and material accumulation in the system.

□

Definition 4-3: Constraint Controlled Variables

The constraint controlled variables are the variables which are to be controlled in order to ensure that process constraints are not violated.

□

The primary controlled variables are normally obtained from the set of dominant variables relating to the key performance measures. Because of the interaction among the dominant variables, it becomes *unnecessary* to control all of the dominant variables. Thus, the set of primary controlled variables $Y_{CV,P}$ is normally a subset of the total dominant variable set Ω_T i.e. $Y_{CV,P} \subset \Omega_T$.

The controlled variables for achieving inventory control purposes can be liquid levels and pressures. Meanwhile, the controlled variables for achieving constraint control objectives can be compositions, temperatures, pressures, pH, etc. Unlike the

primary controlled variables, it is relatively straightforward to identify the inventory and constraint controlled variables from process knowledge and experience.

Bear in mind that the key feature that distinguishes the primary controlled variables from the inventory or constraint controlled variables lies in the way by which they can be identified. Unlike inventory and constraint controlled variables which can be identified directly via process knowledge or experience, it is very difficult to identify the primary (dominant) controlled variables corresponding to a given set of overall (implicit) performance measures based solely on process knowledge.

As an illustration, let consider a process system comprising a tubular (exothermic) catalytic reactor and a distillation column. Process knowledge can be viewed to come from two important sources which are (1) unit operation knowledge and (2) process chemistry. From unit operation knowledge we can identify that the important constraint variables are the reactor hotspot temperature, maximum column pressure, maximum product impurity and maximum or minimum vapour flowrate in the column. From process chemistry, let say we know that the catalyst will disintegrate when the temperature is above certain threshold limit. All of the above variables should constitute the process constraints which must be addressed by the constraint control objectives. Now, an important question is, what are the other variables which must be controlled in order to achieve the *optimum profit objective* for the plant i.e. overall (implicit) performance measure? Obviously we cannot answer this question directly based on our process knowledge. Notice that, the above mentioned constraint variables will probably remain the same if we use two distillation columns instead of one. However, the corresponding controlled variables to achieve the optimum profit will likely to change because these primary controlled variables depend on the nature of interlinked units. Or suppose that we use the fluidized bed reactor instead of tubular reactor but still using the same catalyst, then process chemistry of the catalyst dictates that reactor the temperature is still one of the important process constraints i.e. too high reactor temperature can lead to catalyst degradation. But this will lead to different primary controlled variables, which remain unknown as far as process knowledge is concerned. There is no substitute to good process knowledge in the identification of constraint controlled variables. But one needs a systematic tool to help in the identification of primary controlled variables.

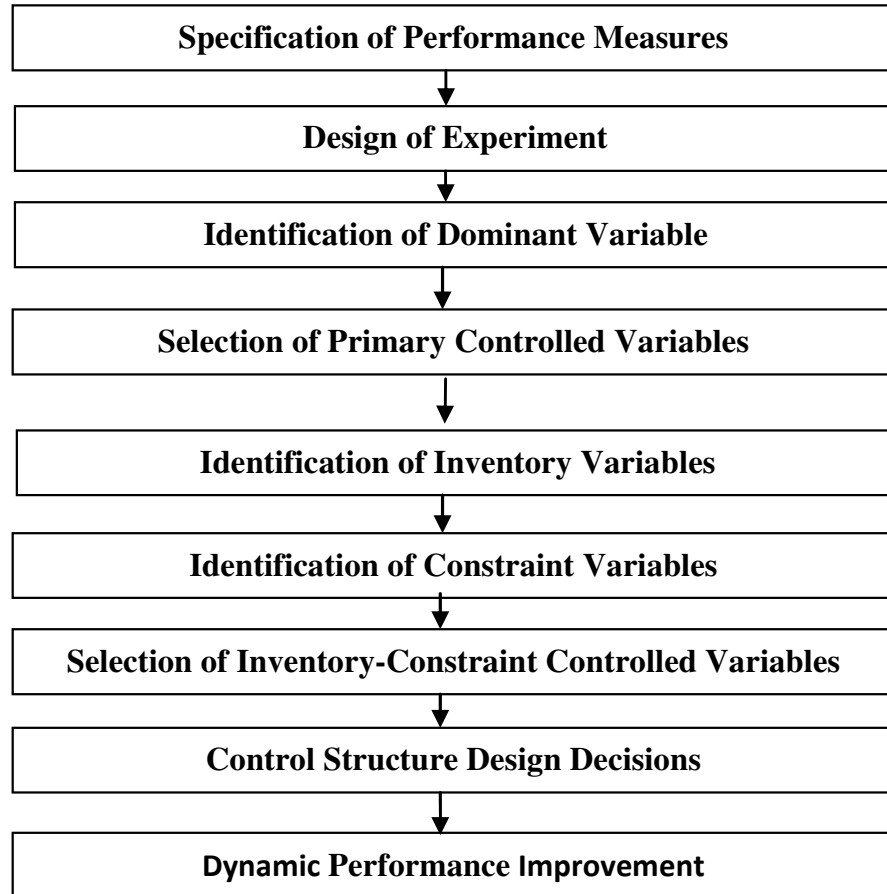


Figure 4-1: Key steps in complete partial control design methodology

4.4 PCA-based Control Structure Design Methodology: Application of Partial Control Framework

Figure 4-1 shows the key steps in the complete partial control design. There are 9 key steps comprising the methodology where the first 4 steps focus on the basic partial control design, which aims to determine the primary controlled variables corresponding to the overall operating objectives. Steps 5 to 7 focus on the determination of suitable controlled variables to achieve the inventory and constraint control objectives. Step 8 addresses the selection of manipulated variables, controller pairings and controller

tuning. Lastly Step 9 aims to enhance the dynamic performance of the overall control system.

Remark 4.1:

In some methodologies such as the 9-step procedure and self-optimizing control, it is viewed as necessary to identify the control degree of freedom (degree of freedom analysis) after the specification of control objectives. Unlike in these methodologies, in the proposed methodology (Figure 4-1) the degree of freedom analysis is embedded in the Step 8. The reason for this is that in partial control normally the number of inputs is very small such that the degree of freedom analysis can be very simple and straightforward. Thus, it is not considered as one of the major issues in the context of partial control structure.

□

More detailed description about each step depicted in Figure 4-1 is as follows:

4.4.1 Determination of Overall Performance Measures

There are 2 key objectives at this step:

- i. Specify the performance measures/overall operating objectives Φ .
- ii. Specify the maximum allowable variations (i.e. $\Delta\Phi_{max}$) of the performance measures in the face of (anticipated) external disturbance occurrence.

Remark 4-2:

Final control structure (i.e. which variables to be controlled and how many controlled variables) depends strongly on the selected performance measures. The main objective at this step is to determine the performance measures which are related to the overall plant objectives such as, optimum profit, minimum energy consumption and optimum trade-off between two certain performance measures. These control objectives are normally implicit functions of the process variables.

□

4.4.2 Design of Experiment (DOE): Plant Data Generation

The main objective is to generate plant *data* which contain *significant information* regarding the performance measures of interest. Two important issues are the determination of:

- i. Set of inputs U_E for design of experiment.
- ii. Magnitude of inputs perturbations ΔU_E .

Process knowledge and experience can be adopted in the process to identify the suitable set of inputs U_E for the design of experiment (DOE). The perturbation magnitude ΔU_E should be large enough such that, the resulting dataset contains some *outliers*.

One type of design of experiment that can be employed is the factorial design for small number of inputs and fractional factorial design for larger number of inputs. The inputs used can be the manipulated variables (i.e. flows) or known disturbances (e.g. temperature, pH, concentration) or a combination of some manipulated variables and some measured disturbances.

4.4.3 Identification of Dominant Variables

Successive dataset reductions using Principal Component Analysis (PCA) are applied to the matrix of *dataset X* (see Chapter 3). Note that, the *dominant variable criteria* must be completely fulfilled at each stage of dataset reduction until the critical level of dataset reduction is reached i.e. the *successive dataset reduction condition* is applied.

We need to specify the threshold value (v_{cric}) for the sum of variances of the first and second principal components for the case where 2D-plot of PCA is used. This value is used as an indicator whether we already reach the critical dataset reduction level. The recommended minimum v_{cric} should be $\geq 80\%$. When the value of v_{cric} is too small, then this can lead to an apparently too many dominant variables i.e. some of the variables are non-dominant.

4.4.4 Selection of Primary Controlled Variables

There are two key questions to be answered at this stage which are:

- 1) Which dominant variables to be controlled?
- 2) How many dominant variables to be controlled?

4.4.4.1 Primary Controlled Variable (PCV) Criteria

The following *Primary Controlled Variable (PCV) criteria* can be used as a guideline in selecting which dominant variables to be controlled:

1. Select the dominant variable/s with the largest (steady-state) influence on the performance measure (we can use CI to rank the dominant variables).
2. For a serial case, select the dominant variable/s in the last stage (downstream) because this implies rejection of most of the disturbance effect i.e. if upstream variable is controlled, then the effect of disturbance that enters through the same point/stage as another variable downstream will be poorly rejected.
3. Select a subset of dominant variables that lead to the most favorable pairings e.g. diagonal RGA elements closed to unity.
4. Select a variable which leads to fast disturbance rejection. This means that we need to compromise between strong steady-state influence (criteria 1) and fast dynamic response. Note that, prior process experience and knowledge regarding the process can be used to identify the inputs which have fast or slow dynamics. Additionally, preliminary simulation study can be adopted in order to find input candidates which have the fast dynamics.

4.4.4.2 PCV Criteria 1 – Relation to Closeness Index

With regard to the first PCV criteria, the selection of controlled variables from the subset of dominant variables can be done based on the ranking of dominant variable influence on performance measure of interest. The ranking of a dominant variable y_i with respect to a certain performance measure ϕ_p can be quantified by its *closeness index* δ_{ip} as described previously in Chapter 3.

Remark 4-3:

In some cases, the rank of the dominant variables is too close to one another i.e. their closeness index values are close to each other. As such, the controlled variable/s can be selected on the basis of dynamic influence on a particular performance measure of interest. In other words, control the dominant variable which has the fastest dynamic influence on the performance measure.

□

4.4.4.3 Determination of Number of Primary Controlled Variables via I_{DV}

With respect to the second key question, it is always desirable to control as small as possible the number of dominant variables. The reason is that, the smaller the number of controlled variables the simpler is the control system. Furthermore, some of the manipulated variables must be reserved for the inventory and constraint control objectives.

To determine the number of primary controlled variables, the *dominant variable interaction index* I_{DV} can be adopted (see Chapter 3). In general, if the elements of I_{DV} are small, then this implies that it is sufficient to control only one or two of the dominant variables i.e. one or two primary controlled variables required. On the other hand if the elements are quite large, then we need to control one or two more extra dominant variables. The procedure of assessing the number of primary controlled variables is as follows.

4.4.4.4 Case 1: Single Performance Measure-Multiple Dominant Variables

For the case of single performance measures with n number of dominant variables, the dominant variable interaction index I_{DV} is given by a column vector as:

$$I_{DV} = \begin{bmatrix} \delta_1 \\ \delta_2 \\ \vdots \\ \delta_n \end{bmatrix} \quad 4-1$$

Algorithm

1. Select the strongest (minimum element) dominant variable $y_k \in \Omega$, $k \leq n$.
2. Check the element of k -row of I_{DV}
3. If $I_{DV}|_k < \delta_{max}$, then it is sufficient to control only y_k .
4. Else, select the second strongest dominant variable $y_l \in \Omega$, $l \leq n$ as follows:
 - i. Calculate the closeness index values of y_k in the directions of other dominant variables (not including δ_{kk}) i.e. $\delta_{k1}, \delta_{k2}, \dots, \delta_{kn}$.
 - ii. Choose the next controlled variable y_l such that δ_{kl} is the largest.
 - iii. Calculate the sum of I_{DV} elements excluding the controlled variables i.e.

$$\Lambda_{kl} = \sum_{i=1, i \neq k, l}^n \delta_i$$

- iv. Take an average closeness index excluding the controlled variables i.e.

$$\bar{\delta}_{kl} = \frac{\Lambda_{kl}}{n}$$

5. If $\bar{\delta}_{kl} < \delta_{max}$, then it sufficient to control only y_k and y_l . Else repeat Steps 4 to 5.

□

Remark 4-4:

Except for the case of strong interaction among the dominant variables where $I_{DV}|_k < \delta_{max}$, it is quite difficult to estimate exactly how many dominant variables should be controlled for the case of weak interaction. Therefore, one alternative way to decide the number of primary controlled variables for the case of weak interaction is via simulation i.e. whether more than one dominant variables should be controlled depends on whether the performance specification is met or not. If not, one needs to control the next (second) strongest dominant variable and a simulation is then performed to evaluate whether controlling 2 dominant variables is sufficient or not. This continues if the performance

objectives are still not achieved. Of course, this is a rather tedious task as we need to iteratively pre-design the controller for the simulation study.

□

Remark 4-5:

Here δ_{max} is a small positive value that is less than unity (heuristically chosen between 0.05 and 0.15). Thus, in general if the value of the closeness index $\delta_{ij} > 0.15$, then this implies a rather weak correlation between the variable y_i and y_j .

□

4.4.4.5 Case 2: Multiple Performance Measures-Multiple Dominant Variables

For the case of m number of performance measures with n number of dominant variables, the dominant variable interaction index I_{DV} is given by a matrix of n rows and m columns:

$$I_{DV} = \begin{bmatrix} \delta_{11} & \delta_{12} & \dots & \delta_{1m} \\ \delta_{21} & \delta_{22} & \dots & \delta_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \delta_{n1} & \delta_{n2} & \dots & \delta_{nm} \end{bmatrix} \quad 4-2$$

Algorithm

1. Select the strongest dominant variable $y_i \in \Omega, i \leq n$, which has the strongest effect on majority of the performance measures.
2. Check the i^{th} row ($I_{i,max}$) elements of I_{DV} matrix.
3. If $I_{i,max} < \delta_{max}$, then it is sufficient to control only y_i . Where $I_{i,max}$ is given by

$$I_{i,max} = \max_{\delta_{ij}|j=1,2..m} (I_{DV}|_i) \quad 4-3$$

Read: find the maximum value δ_{ij} in the i^{th} row of the matrix I_{DV} .

4. Otherwise, find the next strongest dominant variable $y_k \in \Omega, k \leq n$ which has the largest effect on most of the performance measures. Find the k^{th} row with largely small values of closeness index δ_{kj} , where $j = 1, 2 \dots m$.
5. Check for the maximum element within i^{th} and k^{th} rows i.e. $I_{ik,max}$.
6. If $I_{ik,max} < \delta_{max}$, then it is sufficient to control only y_i and y_k .

$$I_{ik,max} = \max_{\delta_{ij}, \delta_{kj} | j=1,2..m} \left[\begin{array}{c} \min_{\delta_{l1}, l=i,k} (I_{DV} |_{i,k}^1), \min_{\delta_{l2}, l=i,k} (I_{DV} |_{i,k}^2), \dots \\ \min_{\delta_{lm}, l=i,k} (I_{DV} |_{i,k}^m) \end{array} \right] \quad 4-4$$

Read: find the maximum value of closeness index among the minimum values of closeness index within the columns involving the i^{th} and k^{th} rows in the I_{DV} matrix.

7. Otherwise, repeat steps 4 to 6, for example, for the case where 3 controlled variables are required. First, find the next strongest dominant variable $y_q \in \Omega, q \leq n$, which has the next largest effect on majority of the performance measures. Then, repeat Step 4 by checking for the maximum element within i^{th} , k^{th} and q^{th} rows i.e. $I_{ikq,max}$. If $I_{ikq,max} < \delta_{max}$, then it is sufficient to control only $\{y_i, y_k, y_q\}$. Where

$$I_{ikq,max} = \max_{\delta_{ij}, \delta_{kj}, \delta_{qj} | j=1,2..m} \left[\begin{array}{c} \min_{\delta_{l1}, l=i,k,q} (I_{DV} |_{i,k,q}^1), \min_{\delta_{l2}, l=i,k,q} (I_{DV} |_{i,k,q}^2), \dots \\ \min_{\delta_{lm}, l=i,k,q} (I_{DV} |_{i,k,q}^m) \end{array} \right] \quad 4-5$$

8. If $I_{ikq,max} < \delta_{max}$, so it is sufficient to control only 3 dominant variables. Otherwise, repeat Steps 4 to 6.

□

Remark 4-6:

For two controlled variables, $\min_{\delta_{ij}} (I_{DV} |_{i,k}^j)$ in Eq. 4-4 means that to find the minimum element (closeness index) of I_{DV} within j^{th} column and involving only i^{th} and k^{th} rows. Similarly for three controlled variables, $\min_{\delta_{ij}, l=i,k,q} (I_{DV} |_{i,k,q}^j)$ in Eq. 4-5 means that to find the minimum element of I_{DV} within j^{th} column involving only i^{th} , k^{th} and q^{th} rows.

□

4.4.5 Identification of Inventory Variables Y_I

Typical inventory variables are liquid level and pressure. Thus, this type of variables is very easy to identify based on minimum knowledge and experience. Here, identify all variables (i.e. liquid levels or pressures) which fall within the inventory category i.e. Y_I . Next, rank the importance of the inventory variables. For example, the vessel or tank which operates closed to maximum capacity should be given priority over other tanks which operate further away from their maximum capacity. Also, the liquid level in reactor should be ranked above that of liquid level in surge tank. Then, specify the maximum steady-state and dynamic variations of inventory variables in the face of disturbance occurrences, i.e. $\Delta Y_{I,max}^{ss}$ and $\Delta Y_{I,max}^{dyn}$ respectively.

Remark 4-7:

The steady-state variation or offset in the variable is the difference between its nominal (setpoint) value and its new steady-state value in the face of external disturbance occurrence. Meanwhile, the dynamic variation in a variable is equivalent to either peak value or minimum value during its transient response. It is important that the peak value during the transient is below the allowable limit, otherwise overflow might occur.

□

4.4.6 Identification of Constraint Variables Y_C

The following steps can be applied to identify the constraint variables:

- i. First, based on the unit operation knowledge plus the physical and chemical knowledge about the bio-chemical components used, identify all the variables (Y_C) that relate to the process constraints characterizing each unit or equipment, which makes up the entire plant. Note that, the process constraints normally form the so-called *operating window* within which the plant must operate to ensure safe, smooth, reliable and profitable operation.

- ii. After identifying all the variables relating to the process constraints, rank the importance of the constraint variables.
- iii. Finally, specify the maximum allowable steady-state and dynamic variations in the face of disturbance occurrence, i.e. $\Delta Y_{C,max}^{ss}$ and $\Delta Y_{C,max}^{dyn}$ respectively.

Note that, the maximum dynamic variation could be either the maximum peak or minimum value during the transient response. Since the peak value during transient can be damaging to the equipment, it is important to ensure that the maximum dynamic variation (e.g. maximum excursion of reactor temperature) of a constraint variable remains within allowable limit of the equipment involved.

Detailed analysis might be required for complex units such as bioreactor, exothermic catalytic reactor and multi-component distillation column. Furthermore, some of the variables that relate to the process constraints might belong to the inventory group of variables. For example, liquid level in reflux drum should not be allowed to fall below certain limit, otherwise the cavitation of pump below the drum will occur and damage the pump. This in turn can lead to unreliable operation or even unsafe operation. Therefore, in this case the liquid level in the reflux drum serves as both inventory and constraint control objectives. Moreover, some of the constraint variables might also belong to the dominant variable set or the primary variable set. For example, the bioreactor temperature may have strong influence on productivity (overall performance measure) and at the same time it is also a constraint variable i.e. high temperature can kill the microbes. Thus, bioreactor temperature serves as both dominant and constraint variable.

4.4.7 Selection of Inventory-Constraint Controlled Variables

Once the candidates for inventory and controlled variables (sets of Y_I and Y_C) are identified, the next tasks are to determine which of the constraint variables should be controlled. Note that, just like in the case of dominant variables, we do not need to control all of the inventory and constraint variables because they are normally interrelated. Thus, this step is very crucial where the main tasks are to determine:

1. Inventory ($Y_{CV,I}$) and constraint ($Y_{CV,C}$) controlled variables from Y_I and Y_C respectively, where $Y_{CV,I} \subset Y_I$ and $Y_{CV,C} \subset Y_C$.
2. Sufficient number of inventory and constraint controlled variables required.

To resolve the first task, the previously mentioned PCA-based method can be adopted in order to gain insight about the nature of the interaction among the inventory-constraint variables. Meanwhile, the second task can be handled via the variable-variable interaction index (I_{VV}).

4.4.7.1 Inventory-Constraint Controlled Variables (ICCV) Criteria

The following criteria can be used as guidelines for the selection of inventory-constraint controlled variables:

1. When two or more variables are strongly correlated, then select the most important variables based on their ranking.
2. When two or more variables are strongly correlated, then select the variables which are easy to measure.
3. When two or more variables are strongly correlated, then select the variables which are most susceptible to disturbances.
4. Select a set of variables that lead to the most favourable pairing i.e. diagonal elements of RGA closed to unity.

With respect to the second task, we want to control sufficient number of variables such that, the variations in Y_I and Y_C are acceptable in the face of disturbance occurrence, i.e.:

$$\begin{aligned} \text{Inventory variables variations: } & \begin{cases} \Delta Y_I^{ss} \leq \Delta Y_{I,max}^{ss} \\ \Delta Y_I^{dyn} \leq \Delta Y_{I,max}^{dyn} \end{cases} \\ \text{Constraint variables variations: } & \begin{cases} \Delta Y_C^{ss} \leq \Delta Y_{C,max}^{ss} \\ \Delta Y_C^{dyn} \leq \Delta Y_{C,max}^{dyn} \end{cases} \end{aligned}$$

To determine the number of inventory-constraint controlled variables, we could adopt the *variable-variable interaction* (I_{VV}) array, which is the extension of the

dominant variable interaction array (I_{DV}) previously mentioned in this chapter. Of course, rather than calculating the closeness index between variable and performance measure (dominant variable case), we need to compute the closeness index between variables. Then, use the variable-variable closeness index values to form the matrix of variable-variable interaction array i.e. I_{VV} . From the values of elements in I_{VV} , we can estimate the sufficient number of variables that should be controlled in order to ensure acceptable steady-state and dynamic variations of the inventory-constraint variables.

4.4.7.2 Variable-Variable Interaction Index I_{VV}

For n constraint and inventory variables (i.e. $Y_C \cup Y_I$), the variable-variable interaction array I_{VV} can be written as:

$$I_{VV} = \begin{bmatrix} \delta_{11} & \delta_{12} & \dots & \delta_{1n} \\ \delta_{21} & \delta_{22} & & \delta_{2n} \\ \vdots & & \ddots & \vdots \\ \delta_{n1} & \delta_{n2} & \dots & \delta_{nn} \end{bmatrix} \quad 4-6$$

Note that, I_{VV} is a square matrix. Since the closeness index of a variable with respect to its own is zero i.e. $\delta_{ij} = 0, i = j$, then the I_{VV} can be expressed as follows:

$$I_{VV} = \begin{bmatrix} \mathbf{0} & \delta_{12} & \dots & \delta_{1n} \\ \delta_{21} & \mathbf{0} & & \delta_{2n} \\ \vdots & & \ddots & \vdots \\ \delta_{n1} & \delta_{n2} & \dots & \mathbf{0} \end{bmatrix} \quad 4-7$$

4.4.7.3 Screening of Inventory-Constraint Controlled Variables via I_{VV}

Algorithm

1. Choose the most critical constraint variable $y_i \in Y_C \cup Y_I, i \leq n$ as controlled variable.
2. Check the maximum element of i^{th} row i.e. $I_{i,max}$
3. If $I_{i,max} < \delta_{max}$, then it is sufficient to control only y_i . Where

$$I_{i,max} = \max_{\delta_{ij}|j=1,2..n} (I_{VV}|i) \quad 4-8$$

Read: find the maximum value δ_{ij} in the i^{th} row of the matrix I_{VV} .

4. Otherwise, control the next most important variable $y_k \in Y_C \cup Y_I, k \leq n$ where this variable shows weak correlation with y_i i.e. $\delta_{ik} > \delta_{max}$.
5. Check the maximum element of i^{th} and k^{th} rows $I_{ik,max}$. Where:

$$I_{ik,max} = \max_{\delta_{ij}, \delta_{kj} | j=1,2..n} \left[\begin{array}{c} \min_{\delta_{l1}, l=i,k} (I_{VV}|_{i,k}^1), \min_{\delta_{l2}, l=i,k} (I_{VV}|_{i,k}^2), \dots \\ \min_{\delta_{lm}, l=i,k} (I_{VV}|_{i,k}^n) \end{array} \right] \quad 4-9$$

Read: find the maximum value of closeness index among the minimum values of closeness index within the columns involving the i^{th} and k^{th} rows in the I_{VV} matrix.

6. If $I_{ik,max} < \delta_{max}$, then it is sufficient to control only y_i and y_k .
7. Otherwise repeat Steps 4 to 6.

□

4.4.8 Control Structure Design Decisions

There are 4 main tasks involved in this step as follows:

- 1) Selection of manipulated variables from the available inputs (control degree of freedom analysis).
- 2) Determination of manipulated-controlled variables pairings using RGA analysis (minimum requirement for simplicity).
- 3) Selection of control law i.e. P-only or PI or PID controller. More advanced controller algorithms can also be considered if the process is very difficult to control using simple PID type controller.
- 4) Controller tuning to meet the desired dynamic responses or control criteria.

Selection of Manipulated Variables Set

Note that, the selection of manipulated variables set (U_{MV}) in partial control is not as critical as the selection of controlled variables set (Y_{CV}). The reason is that, for partial control normally there are only a few suitable inputs which can be manipulated i.e. limited number of control degree of freedom. Thus, most of the time we will use all of

the available inputs as manipulated variables – selection is not an option in this case. However, in the case where there are less number of manipulated variables required than the control degree of freedom, we can employ a few techniques for selection of U_{MV} .

One of the techniques that could be applied to select the U_{MV} from a large number of inputs is the Single-Input Effectiveness (SIE) described in (Cao and Rossiter 1997). Other method which can be used as a guidance to select the suitable manipulated variables is the Morari Resiliency Index (MRI) (Morari 1983). The MRI is a measure of the inherent ability of the control structure to handle disturbances. The larger the value of MRI, the more resilient is the control structure.

Controller Pairings

The selection of controller pairings in partial control is relatively simple as compared with that of more complex control strategies with larger number of controlled variables; in partial control strategy only a few controlled variables are adopted leading to less tedious task of selecting the suitable controller pairings. In general, for simplicity one can always adopt the simple RGA analysis in the selection of controller pairings.

Note that for the controller pairing, one can also adopt more rigorous analysis such as, the dynamic RGA (DRGA), performance RGA (PRGA). For more detail regarding controller pairings readers can refer to (Hovd and Skogestad 1993).

Controller Tuning

Simple and practical method for the controller tuning for multivariable process can be found in (Luyben 1986). For the controller tuning for the multi-loop SISO design, one can use the trial-and-error method based on Ziegler-Nichols tuning because it is simple to implement. Other methods which can be adopted for tuning of PI/PID controllers are as proposed in Lee, Cho and Edgar (1998) and Zhang, Wang and Åström (2002).

Remark 4-8:

Note that, we will not discuss further in this thesis regarding the use of more rigorous analysis for the selection of manipulated variables, controller pairings and controller tunings. For simplicity the selection of manipulated variables is based on the process

knowledge (i.e. with minimum mathematical analysis) while controller pairings is done via the simple RGA analysis. Therefore, the focus of the research work described in this thesis is on the most critical step (and the least studied aspect) of partial control design, which is the selection of controlled variables.

4.4.9 Dynamic Performance Improvement

The last step is to enhance the dynamic performance of the complete partial control design against disturbances. This step is necessary when the dynamic performance of the partial control strategy is still unacceptable, for instance, the recovery of the performance measures (e.g. yield and productivity) is too slow.

There are various strategies which can be adopted at this stage, such as the PID enhancement techniques i.e. cascade, ratio and feedforward control strategies. Additionally, the unused manipulated variables (i.e. remaining input degree of freedom) can also be used to control extra variables, which could further improve the dynamic performance. For the case when the control-loops interactions are too serious, then one can design the decoupler in order to reduce the loops interaction.

4.5 Discussion on Control Structure Design Approach

Why unit operation approach to plantwide control design works? Recall that in this thesis, we divide the operating objectives into three broad category as (1) overall operating objectives, (2) inventory objectives, and (3) constraint objectives. Notice that, most of the operating objectives are attached to the last two control objectives. Interestingly, the vast majority of the variables related to these two objectives can be identified directly from the *unit operation knowledge* i.e. they are the explicit functions of the process constraint variables in most cases.

On the other hand, the number of overall operating objectives which are the implicit functions of the process variables is much smaller than that of combined inventory and constraint objectives. Therefore, it is *intuitively* clear why the unit operation approach work in plantwide control design because the majority of the objectives are related to the constraint and inventory control objectives. Furthermore, the stability which is the most

basic requirement for the process plant operation is frequently governed by the constraint and inventory control objectives, and not by the overall operating objectives.

Since the large majority of operating objectives consist of inventory and constraint types, it seems that one can only focus on these two types of objectives in order to resolve the plantwide control problem. *Thus, an important question becomes why we need to incorporate the overall operating objectives in the plantwide control design at all?*

The answer to this question lies in the idea of profit optimization of a process plant requiring the fulfillment of various *implicit* operating objectives, e.g. maximum yield, productivity and minimum energy consumption, etc. While the constraint and inventory control objectives are basic requirements to operate a plant in a safe, smooth and reliable manner, unfortunately fulfilling only these two types of objectives cannot ensure the attainment of optimum profit i.e. optimum plant operation.

As a result, we need to find which variables to be controlled in order to achieve the overall operating objectives, which can ultimately lead to optimum plant operation. These variables which are subset of the dominant variables are called in this thesis as the primary controlled variables. Unlike the inventory and constraint controlled variables, which can be identified based on the unit operation knowledge and experience, the determination of the primary controlled variables is not as straightforward due to their implicit relationship with the overall performance measures. Therefore, we need a sound theoretical framework to address this type of operating objectives i.e. new partial control framework developed in this thesis.

4.6 Summary

In this chapter, a complete partial control design methodology is proposed. The complete partial control design includes: (1) overall operating objectives, (2) constraint control objectives, and (3) inventory control objectives. These three objectives correspond to three classes of controlled variables which are: (1) primary controlled variables from the set of dominant variables (identified via PCA-based technique), (2) constraint controlled variables from the set of constraint variables, and (3) inventory controlled variables, respectively.

It should be remembered that, the existence of variables interaction means that it is not necessary to control all of the candidate (primary, inventory and constraint) variables. Only a few variables are required as controlled variables, and the rest of the uncontrolled variables will be indirectly controlled by virtue of their interaction with the controlled variables. However, this leads to two key questions: which variables should be controlled and how many variables should be controlled?

One way to identify the primary controlled variables is by using the closeness index (CI) – CI is used to rank the importance of dominant variables. Also, we propose a few heuristic guidelines which can further support the decision relating to this task.

Next, we can assess the number of primary controlled variables using the proposed dominant variable interaction array I_{DV} . There are two cases involved: (1) multiple dominant variables with single performance measure, and (2) multiple dominant variables with multiple performance measures. In both cases we have developed the algorithms required in order to apply the I_{DV} for assessing the sufficient number of primary controlled variables.

Unlike the primary variables, the inventory-constraint variables can directly be identified by means of process (i.e. unit operation) knowledge. We propose a few heuristic rules which can be adopted in selecting the inventory-constraint controlled variables. Additionally, we extend the application of the dominant variable interaction array (i.e. to variable-variable interaction array I_{VV}) to assessing the sufficient number of inventory-constraint controlled variables required.

We might be wondering why in the past until now that partial control strategy has worked quite well despite of its heavy reliance on process knowledge and experience? If this is the case, do we really need a systematic tool for implementing partial control? To these questions we provide the following answers.

First, the majority of the operating objectives are of the inventory and constraint types, which largely determine the safe, smooth and reliable operation. As we know that most of the inventory-constraint variables are usually interacted, thus, this means that there is no need to control all of them. But this also means that, we can choose rather arbitrarily the controlled variables, and the chance that the resulting control strategy is *workable* is high due to the variables interaction.

To answer the second question, we need to ask a further question that is, can this control strategy achieve the implicit objectives, such as, the optimum profit, optimal trade-off between yield and conversion, etc? Then, the answer is clearly no because we need a better tool (other than pure heuristic approach) to precisely translate these implicit objectives into a set of feedback-controlled variables (i.e. the heart of CSD problem). In short, the existing approach to partial control though seems to work quite well, it is unlikely that the resulting control strategy is capable of meeting the overall (implicit) operating objectives. Thus, at best this control strategy can only achieve the inventory and constraint control objectives. Therefore, we need a systematic tool to implement partial control strategy such that, we can achieve all 3 types of operating objectives in a systematic and consistent manner.

5 MODELLING, OPTIMIZATION AND DYNAMIC CONTROLLABILITY: TSCE ALCOHOLIC FERMENTATION PROCESS CASE STUDY

5.1 Introduction

Product inhibition is one of the major limitations restricting the achievement of high yield and productivity in fermentation processes. In ethanolic fermentation, the most prevalent practice to reduce the ethanol inhibition is by adopting the so-called extractive fermentation technique as previously described in Chapter 2. Costa et al. (2001) showed that the integration of vacuum flash vessel can significantly increase the ethanol yield and productivity i.e. the technique results in higher productivity than the traditional batch process.

While the study in Costa et al. (2001) focused on the single-stage design, in this thesis we extend this study to the two-stage design. In this case, two bioreactors in series are used instead of using single large bioreactor as in the case of single-stage design. There are 4 major objectives in this chapter which are to:

1. Develop nonlinear modeling of two-stage continuous extractive alcoholic fermentation system.
2. Optimize the operating conditions (i.e. to achieve optimal trade-off between yield and productivity) for two-stage design and compare the result with that of a single-stage design.
3. Develop new framework for dynamic controllability analysis.
4. Compare the dynamic controllability of two-stage design with that of single-stage design.

A major portion of this chapter was published in the Journal of Chemical Product and Process Modelling (Nandong, Samyudia and Tade 2006). One of the main contributions of the work described in this chapter is the novel approach to analyzing the dynamic controllability. This dynamic controllability approach is based on the

integration of the *v-gap* metric, factorial design of experiment and multi-objective optimization concepts.

5.2 Process Description

The two-stage continuous extractive alcoholic fermentation in this study is based on the single-stage design originally proposed by Silva et al (1999). Using the refined kinetic data, Costa et al (2001) had conducted some studies on the optimization and determination of the effective control structure for the single-stage design based on the concept of factorial design and response surface analysis.

A general scheme of the two-stage continuous extractive fermentation coupled with a vacuum flash vessel is shown in Figure 5-1. There are five interlinked units; two bioreactors in series, a centrifuge, treatment tank and vacuum flash vessel. Conventionally, the usual arrangement in industrial process is to have four interlinked bioreactors with measurement made at the entrance of the first bioreactor and at the exit of the last bioreactor. Moreover, the flash vessel is operated in a temperature range between 28°C to 30°C, which is chosen in order to eliminate the necessity for a heat exchanger installation in the bioreactor(Costa et al, 2001).

A small portion of the heavy phase stream (F_C) from the centrifuge is purged out to avoid the accumulation of impurities and dead cells. Also, in the cells treatment unit the cells suspension is diluted with water. Then, sulphuric acid is added to avoid bacterial contamination.

The following assumptions are made in this study:

- A.1** The separation efficiency of yeast cells from the liquid in the centrifuge is 100%. Thus, the concentration of yeast cells in the light phase stream F_E is zero i.e. all yeast cells go to the heavy phase.
- A.2** As an implication of **A.1**, the substrate and product concentrations in F_E and F_C streams are similar to their concentrations in F_2 stream.
- A.3** Dynamics of the treatment tank and flash vessel are very fast as compared to the dynamics of the bioreactors.
- A.4** Well-mixing in both bioreactors.

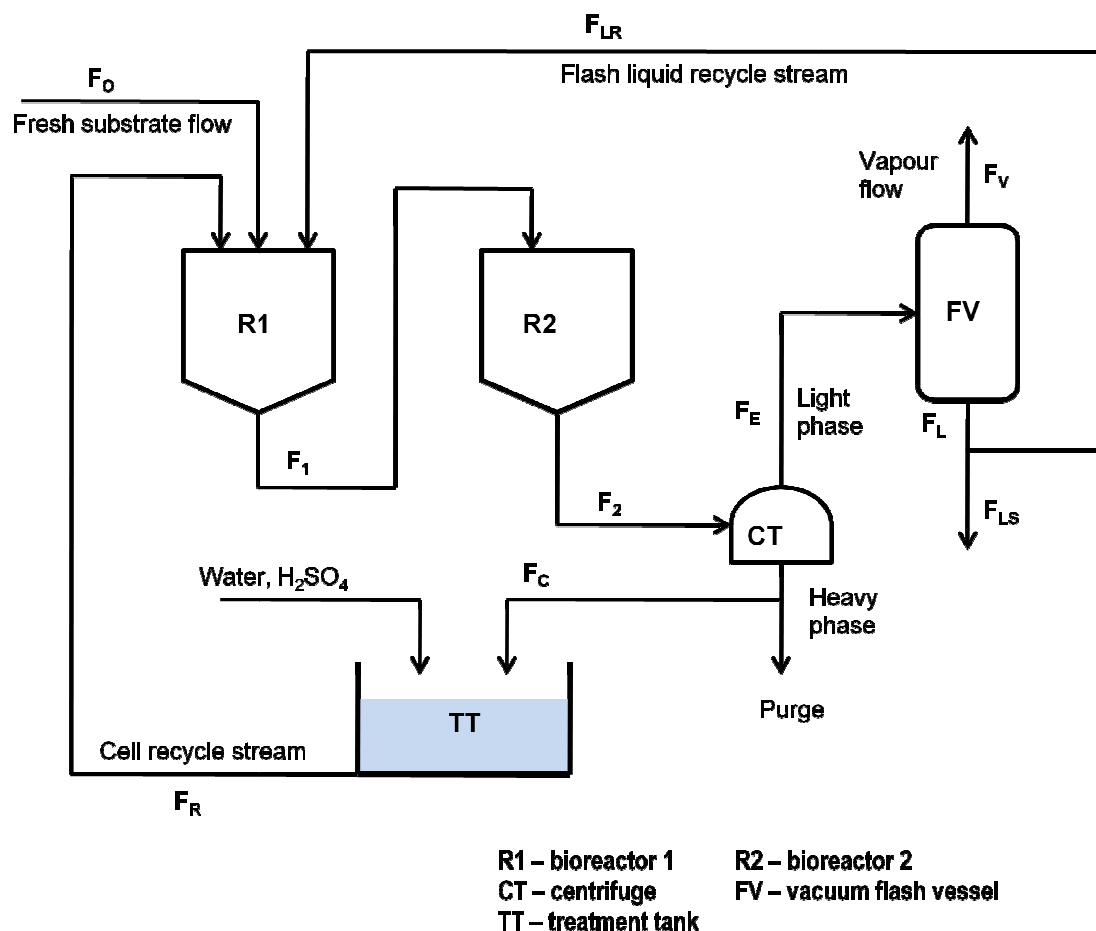


Figure 5-1: Two-stage extractive alcoholic fermentation coupled with vacuum flash vessel

For more detailed information of the modeling approach and kinetic data used in this study, the interested readers can refer to Costa et al (2001). Furthermore, in this study the dynamics of the liquid levels in both fermentors are taken into account in the dynamic controllability analysis. On the other hand in Costa et al (2001), the dynamics of liquid level in the single bioreactor is considered negligible i.e. perfect level control assumption was made.

However, the assumption of perfect level control of liquid level is considered rather unrealistic. Thus, in this thesis we consider the dynamic of liquid level in the bioreactors. The reason is that, in reality to achieve perfect level control in the bioreactors would lead to unacceptable flowrate disturbance to the downstream units such as distillation column. In addition, the control structure design for the system

requires the availability of suitable manipulated inputs (MVs) where in this case the number of MVs is actually much smaller than the number of outputs.

There are only 6 potential MVs, which are:

1. Cell recycle ratio (R)
2. Flash recycle ratio (r)
3. Feed stream (F_o)
4. Exit flowrates from the fermentor 1 (F_1)
5. Exit flowrate from fermentor 2 (F_2)
6. Vapour flowrate from the vacuum flash vessel (F_v)

On the other hand, there are six outputs available for each bioreactor that are:

1. Viable cell concentration (X_v)
2. Dead cell concentration (X_d)
3. Substrate concentration (S)
4. Ethanol concentration (E_t)
5. Bioreactor temperature (T)
6. Fermentor liquid level (L)

Since there are two bioreactors, the total number of outputs available is twelve. Note that, the determination of which outputs to control will be reported in Chapters 6 and 7.

To illustrate that the perfect level control assumption is unrealistic, let consider that the perfect level control in the first bioreactor can be achieved using the exit flowrate (F_1) as the manipulated input. But this stream is actually the inlet flow to the second bioreactor. Consequently, extremely aggressive control action of the liquid level in the first fermentor would lead to heavy fluctuation of F_1 , which in turn becomes serious disturbance to the second bioreactor. Hence, in this study the dynamics of liquid levels in both fermentors would be taken into consideration in the dynamic controllability analysis.

5.3 Modelling of TSCE Alcoholic Fermentation Process

The fermentation process in both bioreactors can be dynamically modelled using a set of differential-algebraic equations (DAEs) coupled with the fermentation kinetic model. It is assumed that bioreactor mixing is ideal (assumption A.4), which implies that the ordinary differential equations can be used to represent the fermentation dynamics. Furthermore, for simplicity and practicality the unstructured kinetic model is adopted rather than the structured metabolic model in order to reduce the computational requirement during the simulation study. The kinetic model takes into account the effects of product, biomass and substrate inhibitions. Also, the effect of temperature on the activity of the living cells is included in the kinetic model.

The following ordinary differential equations are used to represent both bioreactors:

Bioreactor 1

$$A_1 d(L_1 X v_1)/dt = A_1 L_1 (rx_1 - rd_1) - F_1 X v_1 + F_i X v_i \quad 5-1$$

$$A_1 d(L_1 X d_1)/dt = A_1 L_1 (rd_1) - F_1 X d_1 + F_i X d_i \quad 5-2$$

$$A_1 d(L_1 S_1 (1 - X t_1 / \rho))/dt = A_1 L_1 (-rs_1) - F_1 S_1 + F_i S_i \quad 5-3$$

$$A_1 d \left(L_1 E t_1 \left((1 - X t_1 / \rho) + \gamma X t_1 / \rho \right) \right) / dt = \dots$$

$$A_1 L_1 (rp_1) - F_1 E t_1 + F_i E t_i \quad 5-4$$

$$A_1 d(L_1 T_1)/dt = A_1 L_1 (rs_1) (\Delta H_r / (\rho_m C_p)) - F_1 T_1 + F_i T_i \quad 5-5$$

$$A_1 d(L_1)/dt = -F_1 + F_i \quad 5-6$$

Bioreactor 2

$$A_2 d(L_2 X v_2)/dt = A_2 L_2 (rx_2 - rd_2) - F_2 X v_2 + F_1 X v_1 \quad 5-7$$

$$A_2 d(L_2 X d_2)/dt = A_2 L_2 (rd_2) - F_2 X d_2 + F_1 X d_1 \quad 5-8$$

$$A_2 d(L_2 S_2 (1 - X t_2 / \rho))/dt = A_2 L_2 (-rs_2) - F_2 S_2 + F_1 S_1 \quad 5-9$$

$$A_2 d \left(L_2 E t_2 \left((1 - X t_2 / \rho) + \gamma X t_2 / \rho \right) \right) / dt = \dots$$

$$A_2 L_2 (rp_2) - F_2 Et_2 + F_1 Et_1 \quad 5-10$$

$$A_2 d(L_2 T_2)/dt = A_2 L_2 (rs_2) (\Delta H_r / (\rho_m C_p)) - F_2 T_2 + F_1 T_1 \quad 5-11$$

$$A_2 d(L_2)/dt = -F_2 + F_1 \quad 5-12$$

For $j = 1, 2$, the kinetic equations are:

Rate of yeast cell growth:

$$rx_j = \mu_{max} (S_j / (K_s + S_j)) \exp(-K_i S_j) \times \\ (1 - Xt_j / X_{max})^m (1 - Et_j / P_{max})^n Xv_j \quad 5-13$$

Rate of yeast cell death:

$$rd_j = K_{dT} \exp(K_{dp} Et_j) Xv_j \quad 5-14$$

Rate of ethanol formation:

$$rp_j = Y_{px} rx_j + m_p Xv_j \quad 5-15$$

Rate of substrate consumption:

$$rs_j = rx_j / Y_x + m_s Xv_j \quad 5-16$$

The kinetics data adopted in this study can be found in Table 5-1. Furthermore, other algebraic equations describing the system are given as:

$$Xt_j = Xv_j + Xd_j \quad 5-17$$

$$F_i = F_O + F_R + F_{LR} \quad 5-18$$

$$F_{LR} = rF_L \quad 5-19$$

$$F_R = RF_2 \quad 5-20$$

Yield of ethanol produced per maximum theoretical yield is given by:

$$Yield = (F_V Et_v + F_{LS} Et_{LR}) / (0.511 F_O S_O) \quad 5-21$$

Volumetric productivity of ethanol produced is given by:

$$Prod = (F_V Et_v + F_{LS} Et_{LR}) / (V_1 + V_2) \quad 5-22$$

Other algebraic equations for centrifuge and vacuum flash vessel:

$$F_E = F_L + F_V \quad 5-23$$

$$F_L = F_{LR} + F_{LS} \quad 5-24$$

$$F_2 = F_C + F_E \quad 5-25$$

The centrifuge is assumed to achieve perfect solid-liquid separation (assumption A.1), thus, no solid in the light phase. Consequently, this leads to the concentration of cells in the heavy phase to be equal to the wet cell density or maximum concentration (ρ). Thus, the heavy phase stream is simply given by:

$$F_C = (Xv_2 F_2) / \rho \quad 5-26$$

A small portion of heavy phase flow is purged (F_P) and the rest is sent to treatment tank (F_{CT}). Where the flow of the wet cells sent to the treatment tank is given by:

$$F_{CT} = F_C - F_P \quad 5-27$$

Note that, for $j = 1, 2$; the notations used in the modeling are as:

Xv_j	Viable cells concentration in bioreactor j [kg/m ³]
Xd_j	Dead cells concentration in bioreactor j [kg/m ³]
Xt_j	Total cells concentration in bioreactor j [kg/m ³]
S_j	Substrate concentration in bioreactor j [kg/m ³]
S_o	Fresh substrate concentration [kg/m ³]
Et_j	Ethanol concentration in bioreactor j [kg/m ³]
Et_v	Ethanol concentration in vapour phase in flash vessel [kg/m ³]
Et_{LR}	Ethanol concentration in liquid phase in flash vessel [kg/m ³]
T_j	Fermentation medium temperature in bioreactor j [°C]

T_i	Inlet temperature of feed flow into bioreactor I [$^{\circ}\text{C}$]
L_j	Liquid hold-up level of bioreactor j [m]
F_j	Outlet flow rate from bioreactor j [m^3/hr]
F_i	Total feed flow rate to bioreactor I [m^3/hr]
F_O	Fresh substrate flow rate to bioreactor I [m^3/hr]
F_R	Cell recycle flow rate [m^3/hr]
F_{LR}	Liquid flash recycle flow rate [m^3/hr]
F_{LS}	Liquid flash flow rate taken as product [m^3/hr]
F_V	Vapour flash flow rate taken as product [m^3/hr]
F_E	Light phase flow rate from centrifuge [m^3/hr]
F_C	Heavy phase flow rate from centrifuge [m^3/hr]
r	Flash recycle ratio [-]
R	Cell recycle ratio [-]
A_j	Cross-sectional area of bioreactor j [m^2]
V_j	Volume of bioreactor j [m^3]
ΔH_r	Heat of substrate consumption [kJ/kg]
C_p	Specific heat capacity of fermentation medium [kJ/kg. $^{\circ}\text{C}$]
ρ	Wet yeast cells density [kg/ m^3]
ρ_m	Density of fermentation medium [kg/ m^3]

5.4 Design of Experiment of TSCE Alcoholic Fermentation

The extractive alcoholic fermentation process could be optimized using response surface methodology without the need for model simplifications. Hence, the combination of factorial design and response surface methodology provides a convenient alternative to the nonlinear model-based optimization, which is well known to be very time-consuming. However note that, in order to obtain more accurate optimization result, model-based optimization technique should be employed. Here, the optimization based on response surface is adopted in order to be consistent with the previous works (Silva et al 1999, Costa et al 2001).

For the single-stage design, various results of the maximum productivity and yield were reported. Costa et al (2001) reported the highest values of productivity and yield that can be achieved are $21 \text{ kg/m}^3\cdot\text{hr}$ and 82% respectively when the values of fresh substrate concentration, $S_o = 130 \text{ kg/m}^3$, cell recycle ratio, $R = 0.3$, flash liquid recycle ratio, $r = 0.25$ and residence time $t_r = 1.3 \text{ hr}$. These operating conditions correspond to bioreactor volume of 257.4 m^3 .

Using the input values determined by Silva et al (1999): $S_o = 180 \text{ kg/m}^3$, $R = 0.35$, $r = 0.4$ and $t_r = 1.2 \text{ hr}$, Costa et al (2001) showed that the highest productivity and yield are $22 \text{ kg/m}^3\cdot\text{hr}$ and 81% respectively. However, this resulted in the bioreactor volume of 339.8 m^3 .

In the following, we present our results for the two-stage design. Table 5-2 shows the coded factor level for the factorial design of experiment. The chosen nominal operating conditions are corresponding to the values of productivity, yield and conversion of $14.5 \text{ kg/m}^3\cdot\text{hr}$, 82.4% and 86.8% respectively.

From this factorial design of experiment, a set of models as equations (Eq. 5-27, Eq. 5-28 and Eq. 5-29) are produced, where the models relate the productivity, yield and conversions to the most significant input variables in Table 5-2. By using these models, a response shape optimisation is performed, where one of the results is seen in Figure 5-2 and Figure 5-3.

Equations for yield (*Yield*), productivity (*Prod*) and conversion (*Conv*) are given by:

$$Yield = 21.5 + 0.7F_o - 0.46S_o + 109.1R + 126.3r - r(1.3F_o - 0.57S_o) \quad 5-28$$

$$Prod = 118.6 - 0.4F_o - 0.5S_o - 214.6R - 230r + S_o(1.2R + 1.3r - 2.9rR) + r(442R + 0.8F_o) \quad 5-29$$

$$Conv = -7.2 + 0.8F_o - 0.2S_o + 90.2R + r(203 + 1.5F_o) \quad 5-30$$

Table 5-1: Kinetic parameters used in modeling of two-stage continuous extractive alcoholic fermentation system

Parameter	*Expression or value
μ_{max}	$1.57 \exp(-41.47/T) - 1.29 \times 10^4 \exp(-431.4/T)$
X_{max}	$-0.3279T^2 + 26.41T - 191.06$
P_{max}	$-0.4421T^2 + 26.41T - 279.75$
Y_x	$2.704 \exp(-0.1225T)$
Y_{px}	$0.2556 \exp(0.1086T)$
K_S	4.1
m_p	0.1
m_x	0.2
m	1.0
n	1.5
K_{dP}	$7.421 \times 10^{-3}T^2 - 0.4654T + 7.69$
K_{dT}	$4 \times 10^{13} \exp(-41947/[1.987(T + 273.15)])$
ρ	390
δ	0.78

*Data taken from Costa et al. (2001)

Table 5-2: Coded factor level and real values for factorial design ($\pm 25\%$ change from nominal value)

Variable	Level (-1)	Nominal (0)	Level (+1)
F_0 (m ³ /hr)	75	100	125
S_0 (kg/m ³)	112.5	150	187.5
R (-)	0.1875	0.25	0.3125
R (-)	0.30	0.40	0.50

As shown in Figure 5-2, the productivity of bioethanol increases with the increase in flash recycle ratio (r), but at reduced fresh substrate concentration (S_o). In contrast, Figure 5-3 indicates that the yield of bioethanol drops with the increase in r and the decrease in S_o . Hence the productivity and yield show opposite trends to the changes in r and S_o as previously reported in the single-stage design (Silva et al. 1999, Costa et al. 2001). It is important to note that, therefore, the two-stage design exhibits a similar trend in the productivity and yield to that reported of the single-stage design.

Remark 5.1:

Note that, the magnitude of input perturbations used to generate the dataset for response surface analysis is only 20% of the nominal values. The magnitude of input perturbations used in this case is chosen based on the assumption that the system is subject only to disturbances changes (no large setpoints changes occur). In other words, under closed-loop situation in the face of disturbances occurrence the magnitude of variations in the manipulated variables are within this $\pm 20\%$ of input perturbations. Of course, in practice the actual variations in manipulated variables could be larger than this perturbation magnitude if the disturbances are too large or if large setpoints changes occur. In this case however, we assume the disturbances magnitudes are moderate (or setpoint change is not too large) such that the steady-state variations in manipulated variables are within $\pm 20\%$ of their nominal values in the face of disturbances occurrences.

□

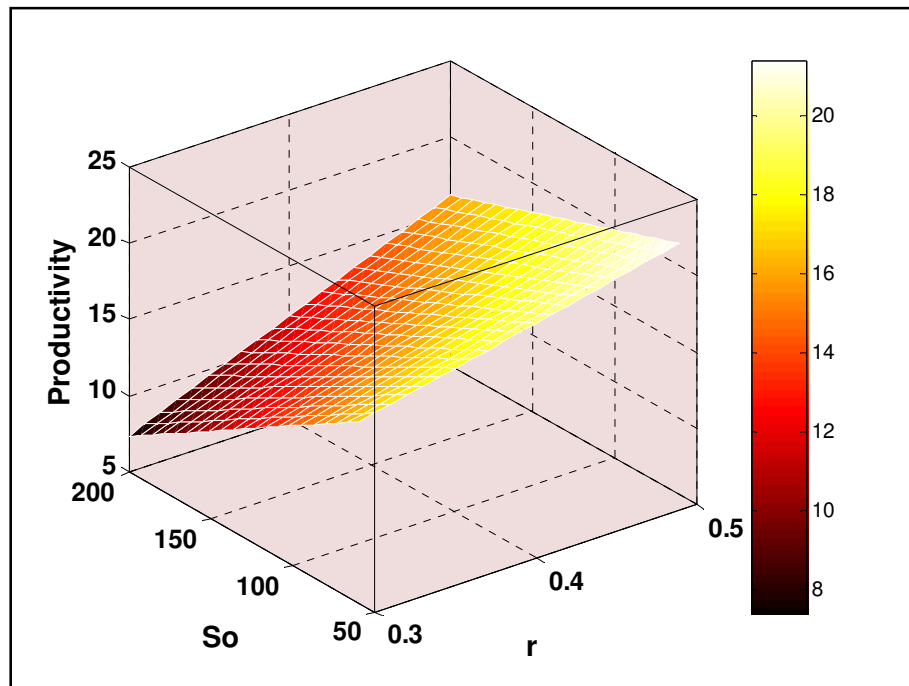


Figure 5-2: Response surface of productivity for $F_o=100 \text{ m}^3/\text{hr}$ and $R = 0.20$

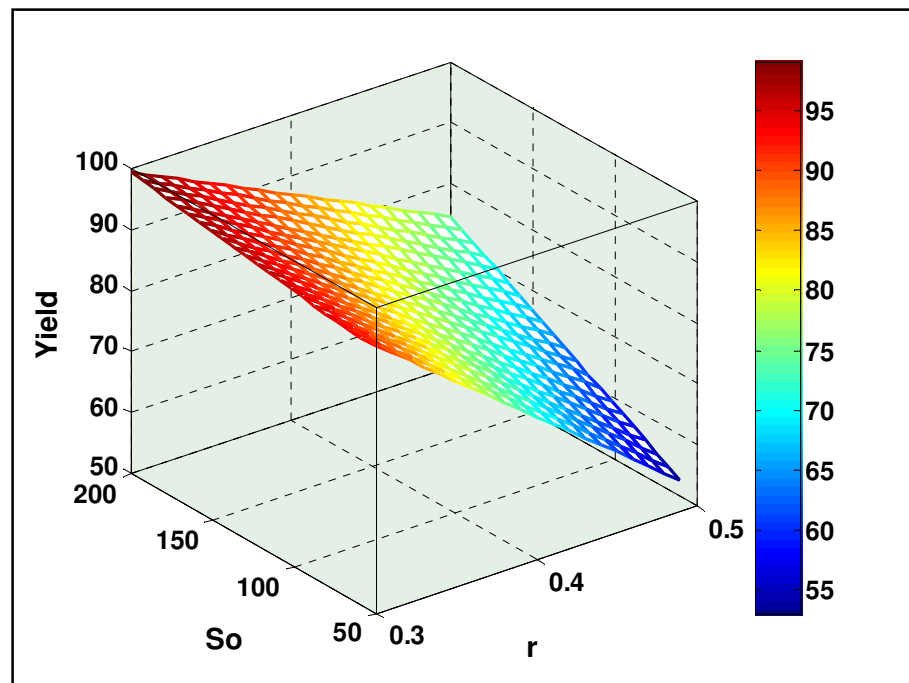


Figure 5-3: Response surface of yield for $F_o = 100 \text{ m}^3/\text{hr}$ and $R = 0.20$

5.5 Optimization of TSCE Alcoholic Fermentation System

Since the *Yield* and *Prod* have opposite trends, it is important to find the optimal trade-off between these two performance measures. To obtain the optimal trade-off between *Yield* and *Prod*, the following cost function is optimized:

$$Y = Yield/Yield_{max} + Prod/Prod_{max} \quad 5-31$$

Where *Yield* and *Prod* are given by (5-27) and (5-28) and $Yield_{max}$ and $Prod_{max}$ are taken to be 90% and 27 kg/m³.hr, respectively. The following optimization problem (**P-5.1**) is solved using Matlab optimization toolbox:

(**P-5.1**)

$$\max_{r, R, V_1, V_2, S_0} (Y)$$

Subject to:

$$M(Y, U) = 0 \quad 5-32$$

$$0.1 \leq r \leq 0.5 \quad 5-33$$

$$0.1 \leq R \leq 0.5 \quad 5-34$$

$$100 \leq S_0 \leq 200 \quad 5-35$$

$$50 \leq V_1 \leq 250 \quad 5-36$$

$$50 \leq V_2 \leq 250 \quad 5-37$$

Note that, Eq. 5-31 corresponds to the steady-state model of the TSCE alcoholic fermentation system. In this optimization, the fresh feed flowrate (F_o) is fixed at constant value of 100m³/hr. Based on the optimization problem (**P.5-1**) for the two-stage design, the optimal trade-off attainable for yield and productivity are 82% and 21 kg/m³.hr respectively. These values correspond to the input values of $S_o = 120$ kg/m³, $R = 0.225$, $r = 0.27$ and $t_r = 1.27$ hr, which results in a total reactor volume of 236 m³. Hence, in term of the maximum achievable yield and productivity, the performances of both single-stage and two-stage designs are comparable.

However at maximum yield and productivity, the two-stage design requires a significantly smaller total bioreactor volume than that required by the single-stage design, i.e. about 8% and 31% smaller than that obtained by Costa et al (2001) and Silva et al (1999), respectively.

Remark 5.2:

It is important to bear in mind that although two-stage design leads to smaller total bioreactors volume than that of the single-stage design, this does not mean that the former is cheaper than the latter. In other words, the capital cost of two small bioreactors can be larger than that of a (single) large bioreactor. So, the decision to proceed with the study of two-stage design in thesis is driven not by the cost but by the complexity of the system. In this case, two-stage design is more complex than the single-stage design, which could offer opportunity to gain more insights into the challenges of bioprocess control design.

□

5.6 Dynamic Controllability Methodology

The main limitation of any steady-state process design is its inability to handle uncertainties and disturbances occurring during the process operation that causes variability in the plant performance (Perkins and Walsh 1996). Various methodologies have been developed for addressing the interactions between process design and process control, such as simultaneous design and control algorithm (Kookos and Perkins 2001), design and control via model analysis (Russel, et al. 2002) and design and control optimization via parametric controllers (Sakizlis, Perkins and Pistikopoulos 2003).

In this work, a simple, sequential methodology of the integrated design and control is proposed. This methodology combines the concepts of the factorial design, *v-gap* metric and robust optimal (loop-shaping) control design to determine whether the process designs (i.e. single-stage or two-stage) have a favourable dynamic operability.

The magnitudes of the input perturbations which are applied to both designs are the same and equal to $\pm 20\%$ of the nominal values. Table 5-3 shows the coded factor level for the single-stage design. The nominal conditions correspond to 82% of yield and 18

kg/m³.hr of productivity. The coded factor level shown in Table 5.4 is for the two-stage design, where its nominal operating conditions correspond to yield and productivity of 84% and 19.4 kg/m³.hr, respectively.

The following algorithm is proposed to compare the dynamic operability of the two designs at the prescribed operating levels. In order to ensure consistency, the nominal operating conditions for each design are chosen such that their yield and productivity are approximately similar.

5.6.1 Preliminaries: v-Gap Metric

Let a linear model $P_i = N_i M_i^{-1} = \bar{M}_i^{-1} \bar{N}_i$, where $N_i, M_i^{-1}, \bar{M}_i^{-1}$ and \bar{N}_i denote the normalized right and left coprime fractional descriptions of P_i (Anderson, Brinsmead and De Bruyne 2002). Further define the following:

$$G_i(s) = \begin{bmatrix} N_i(s) \\ M_i(s) \end{bmatrix} \quad 5-38$$

$$\bar{G}_i(s) = [\bar{M}_i(s) \quad \bar{N}_i(s)] \quad 5-39$$

Following the result of (Vinnicombe 2001), the v-gap metric between two linear (plant) models P_1 and P_2 can be defined as follows:

$$\delta_v(P_1, P_2) = \|\bar{G}_2 G_1\|_\infty \quad 5-40$$

If and only if the $\det\{\bar{G}_2 G_1(j\omega)\} \neq 0 \forall \omega \in (-\infty, \infty)$ and the $wno(\det(\bar{G}_2 G_1)) = 0$; otherwise $\delta_v = 1$. The wno and \det indicate the winding number and determinant respectively. An important property of v-gap is its relationship with the robustness-performance indicator ($b_{p,c}$) of an optimal loop-shaping controller (McFarlane and Glover 1992). For a stable closed-loop system consists of a plant P under the controller C , the general robustness stability margin of the controller can be written as:

$$b_{p,c} = \left(\left\| \begin{bmatrix} P \\ I \end{bmatrix} (I - CP)^{-1} \begin{bmatrix} -C & I \end{bmatrix} \right\|_\infty \right)^{-1} \quad 5-41$$

When $\delta_v(P_1, P_2) < b_{P_1, C}$ where C is a controller designed based on the plant model P_1 then, the controller is guaranteed to be stable for the plant dynamic described by P_2 .

Furthermore, if the value of δ_v is small compared to $b_{P_1, C}$ then, the controller performance will be expected to be comparable for both plant dynamics. It is important to note that, if $\delta_v(P_1, P_2) > b_{P_1, C}$ then, this does guarantee the instability of the controller C when it is used for the dynamic behaviour described by P_2 . However, this will normally lead to performance degradation of the controller.

5.6.2 Description of Uncertainties–Controllability Relationship

The plant uncertainties could be due to various factors, for examples, plant/model mismatch due to unmodelled dynamics of the valves and sensors, unaccounted changes in the dynamics of equipment (time-variant parameters) and disturbances occurrences *e.g.* changes in the raw material compositions.

Figure 5-4a below illustrates the changes in dynamics due to disturbances and process nonlinearities. The linear controllers are presumably designed based on a nominal operating level, P_0 . Due to disturbances the controllers will adjust the manipulated variables (U_1 and U_2) to bring back the process outputs to setpoints. In this respect, it is important to note that if the system is linear then such disturbance occurrence will not change the dynamic behaviour as the manipulated variables change.

Consequently during the course of operation, as the manipulated variables change, the plant dynamic behaviours will also change because of process nonlinearity. The degree of deviation of the perturbed dynamic from the nominal dynamic of the plant depends on the magnitude and direction of input changes, and also the severity of process nonlinearity.

With regard to this type of uncertainty, the question becomes how to measure or quantify the difference in dynamic behaviour between the nominal level and the perturbed levels? Answering this question is important in order to properly design the controller (*i.e.* to make an *optimal trade-off* between performance and robustness) for the pre-selected nominal operating conditions at P_0 in anticipation for the worst-case disturbance scenario.

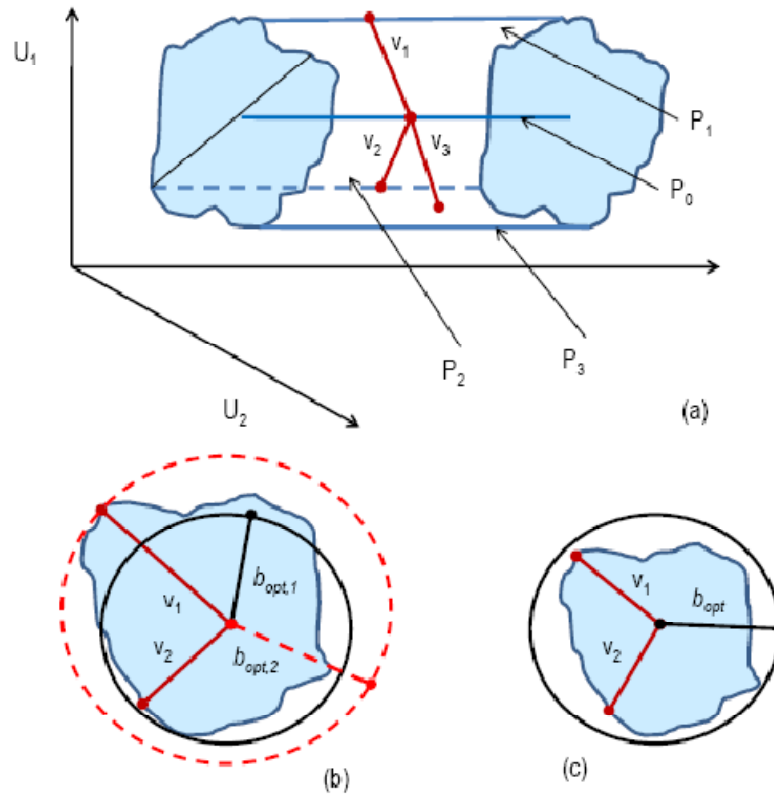


Figure 5-4: Schematic representation of the relationship between dynamic controllability (b_{opt}) and uncertainties (v -gap): (a) perturbed operating levels due to inputs changes, (b) dynamically unfavourable design, and (c) dynamically favourable design

In the proposed dynamic controllability methodology, the distance or difference i.e. $v_1 = \delta_v(P_0, P_1)$ between the nominal dynamic (model) behaviour at P_0 and that of the perturbed model behaviour at P_1 is measured using the concept of v -gap proposed by Vinnicombe (2001).

Another question that needs to be addressed is how well the controller, which is designed based on the nominal model at P_0 cope with the disturbances that cause the change in dynamic behaviour i.e. robustness issue. Obviously using the traditional PID controller, this robustness issue cannot be directly taken into account during its design. Consequently, to address the robustness issue systematically in the methodology, the robust-optimal (loop-shaping) controller proposed by McFarlane and Glover (1992) is

adopted. Based on the loop-shaping controller, the robustness-performance trade-off is indicated by the parameter b_{opt} .

Figure 5-4b and Figure 5-4c illustrate how the proposed methodology could be used to compare the different designs and determine the design with the most favourable dynamic operability. Ideally, it is desirable that all of the distances (v_1, v_2, \dots) to be within the b_{opt} of the loop-shaping controller designed based on the nominal model (see Figure 5-4c).

The plant design as illustrated by Figure 5-4b is not dynamically favourable because most of the perturbed distances are outside the b_{opt} and hence, the stability cannot be guaranteed for this controller in the face of disturbances occurrence. One possible solution is to enlarge the stability margin by increasing the b_{opt} but then this will lead to poor controller performance i.e. sluggish response.

The third important question is how to capture the process nonlinearities? One possible solution is to measure a series of distances between the nominal level and the perturbed levels (i.e. v_1, v_2, v_3, \dots), then to plot the contour line as shown by Figure 5-4b or Figure 5-4c. Note that, (Helbig, Marquardt and Allgower 2000) proposed a method that can be used to measure the process nonlinearities in the opened-loop sense. However, the main limitation of the technique is that the formulation leads to a large, non-convex nonlinear optimization problem. Hence the technique not only requires prohibitive computational effort but also it does not guarantee a global convergence for each distance computed.

As to alleviate the computational effort, the proposed methodology in this chapter adopts the concept of factorial design based on the manipulated variables (MVs) in order to capture the process nonlinearity using the closed-loop metric ($v\text{-gap}$). This leads to a reduced number of distances to be computed, for example, based on 3 MVs the number of distances to be computed is only 8 (i.e. v_1, v_2, \dots, v_8).

Remark 5-3:

One of the key question in measuring the nonlinearity of a given operating point for the multivariable system is that, how do we generate points around the selected nominal operating level such that the result is an accurate assessment of the nonlinearity at that

operating level. Furthermore, how many points that is required to adequately calculate the nonlinearity at this nominal level? In the proposed methodology, the design of experiment concept can be adopted to generate the perturbed points around the specified nominal operating level. This avoids random selection of the perturbed points where if the number is too large it can lead to heavy computational requirement. Thus, in this manner the technique based on the design of experiment not only allows us to generate points in a structurally sound way, but also reduces the number of perturbed points needed for assessing the nonlinearity. Of course, once the perturbed points are obtained, we can conveniently assess the distances between these points and the nominal point using v-gap metric. The next question is can a controller be designed to minimize these distances which is a measure of nonlinearity? If we are comparing two designs A and B for example, obviously we would prefer to choose whichever design that leads to small distances e.g. if a controller can be designed such that the distances of A are largely smaller than that of B, then we should choose A because smaller distances means better controllability property. It is important to note that, to optimally design a controller which minimizes the perturbed distances, we can adopt the multi-objective optimization. Of course, it can be argued that we can also adopt the single-objective optimization which is to minimize the worst case scenario (i.e. the largest distance). However, the drawback of this approach is that while this largest distance is minimized, it could lead to other perturbed distances to exceed the performance limit (see Figure 5-4 for illustration). Therefore, it becomes clear why we choose to adopt multi-objective optimization because we intend to reduce as many as possible the perturbed distances to within the performance limit. Overall, the novelty of the proposed methodology lies in the integration of three concepts: v-gap metric to measure the distance between two points (i.e. model error), design of experiment to generate minimum number of perturbed points for nonlinearity assessment and multi-objective optimization is used to design a controller in order to ensure as many of these perturbed points are brought to be within the specified performance limit.

□

5.7 Algorithm of Controllability Analysis

To perform the analysis of alternative designs, we apply the following procedure:

- Step 1:** Given a set of plant designs and their input-output structures, and, for each design, select the nominal operating level.
- Step 2:** Generate a number of input perturbations about the nominal operating conditions via factorial design i.e. in this case the factorial design is based on three inputs (i.e. R , r and F_o), which will lead to 8 perturbations ($P1, P2, \dots, P8$). Table 5-3 and Table 5-4 show the coded factor level for factorial design of single-stage and two-stage of extractive fermentation processes, respectively.
- Step 3:** Linearize the plant at the nominal operating level and at the perturbed operating levels. These result in 9 linearized models, a linear model at the nominal level ($P0$) and 8 linear models at the perturbed levels ($P1-P8$).
- Step 4:** Apply scaling to the models based on the maximum anticipated changes in inputs and outputs.
- Step 5:** Select weighting (W_e) structure e.g. PI with lead-lag structure, to accommodate the desired closed-loop performance specification. Simple structure with a minimum number of parameters is desirable since this would reduce the computational time.
- Step 6:** Perform the optimization to determine the optimal weight parameters of W_e that minimize the values of $v\text{-gap}$ between the nominal model and perturbed models (or $\delta(P_0 W_e, P_i W_e)$), subject to a specified closed-loop performance within the robust optimal control framework.

Table 5-3: Coded factor level and real values for factorial design (single-stage), $S_o = 170 \text{ kg/m}^3$

Variable	Level (-1)	Nominal (0)	Level (+1)
R (-)	0.24	0.3	0.36
r (-)	0.344	0.43	0.516
F_o (m^3/hr)	80	100	120

Table 5-4: Coded factor level and real values for factorial design (two-stage), $S_o = 130 \text{ kg/m}^3$

Variable	Level (-1)	Nominal (0)	Level (+1)
r (-)	0.2	0.25	0.3
R (-)	0.24	0.3	0.36
F_o (m^3/hr)	80	100	120

5.8 Controllability Analysis – Accommodation of Closed-Loop Performance

To accommodate the desired closed-loop performance in the controllability analysis, the following decentralized input weight is used:

$$W_e = \begin{bmatrix} w_{11} & 0 & 0 \\ 0 & w_{22} & 0 \\ 0 & 0 & w_{33} \end{bmatrix} \quad 5-42$$

Note that in the following case study, we select the manipulated (U_{MV}) and controlled variables (Y_{CV}) as:

$$U_{MV} = \begin{bmatrix} F_o \\ R \\ r \end{bmatrix}, \quad Y_{CV} = \begin{bmatrix} Xv \\ Et \\ L \end{bmatrix}$$

For the two-stage design the output variables to be controlled are that of the second bioreactor i.e. controlled variables are (Xv_2, Et_2, L_2) . Some guidelines regarding the selection of the weighting structure can be found from (Samyudia and Lee 2004). Let us take the weight to have the following form of PI lead-lag structure:

$$w_{jj} = (k_{jj}s + z_{jj})/s(d_{jj}s + 1); j = 1, 2, 3 \quad 5-43$$

Let the vectors of the weighted parameters be $K = [k_{11} \ k_{22} \ k_{33}]^T$, $D = [d_{11} \ d_{22} \ d_{33}]^T$ and $Z = [z_{11} \ z_{22} \ z_{33}]^T$. Then, to find the optimal parameters of the weights minimizing the values of v -gap (Vinnicombe 2001) between the weighted nominal model $P_o W_e$ and that of the perturbed models $P_i W_e$, we can use the multi-objective optimization as given by:

(P-5.2)

$$\min_{K, Z, D} \max_{F_i} (F_i(K, Z, D)), \text{ for } i = 1, 2, \dots, n$$

Subject to the robust optimal performance:

$$b_L \leq b_{opt} \leq b_U \quad 5-44$$

The performance constraints of b_L and b_U are positive scalar values between 0 and 1. In this study, we choose these values to be 0.3 and 0.5 for b_L and b_U , respectively, which are reasonable target of closed-loop performance.

In problem **P-5.2**, n is equal to the number of perturbed operating levels plus the nominal operating level. For example, if 3 inputs are used and based on factorial design, there are 8 perturbed operating levels. Thus $n = 8 + 1 = 9$. Note that, to solve the problem **P-5.2**, multi-objective optimization technique is required. Here, the problem is solved using Matlab optimization toolbox.

Note that, the v -gap between the weighted nominal model P_0W_e and that of the perturbed model P_1W_e is given by:

$$F_i(K, Z, D) = \delta_v(P_0W_e, P_1W_e) \quad 5-45$$

Where $i = 1, 2 \dots 8$ corresponding to the number of perturbed operating levels.

Also note that the value of b_{opt} indicates the *achievable performance* and *robustness* of the feedback controller. The smaller this value, the faster the closed-loop response would be. But, if it is too small the closed-loop system becomes less robust to uncertainty. For a good compromise between performance and robustness, this value is normally chosen to be around 0.3. The optimization based on the problem **P.5-2** is nonlinear. So, its convergence to a global solution cannot be guaranteed. In addition, there is no unique set of values of W_e that actually minimizes the worst v -gap and at the same time fulfils the specified performance b_{opt} .

5.9 Results and Discussion

Figure 5-5 and Figure 5-6 show the step responses (open-loop case) of the ethanol concentration (Et) to the fresh substrate flowrate F_o at different operating levels based on the linearized models. The response at $P1$ in the single-stage design indicates large difference from that at the nominal point $P0$. This is expected from the analysis presented in Table 5-5, which shows that the v -gap (i.e. measure of model error) between $P0$ and $P1$ is 1.0 (maximum). Hence, this confirms a large difference (or error)

between the nominal and perturbed models i.e. strongly nonlinear behaviour in the $P1$ direction.

However, there is no clear-cut relation between open-loop responses and $v\text{-gap}$ values i.e. $v\text{-gap}$ value could be small (indicate close similarity between nominal and perturbed models) but their open-loop responses could be very different. For example, Table 5-6 shows that the $v\text{-gap}$ between $P0$ and $P1$ (0.78) is larger than that between $P0$ and $P3$ (0.385) and yet, open-loop responses of $P1$ and $P0$ looks more comparable than that of $P3$ and $P0$ as shown in Figure 5-6. Table 5-5 and Table 5-6 indicate the $v\text{-gap}$ values of the eight perturbed models from the nominal model for the single-stage and two-stage designs, respectively.

Note that, the case of *not weighted* meaning that no performance specification is imposed to the process. In this case, the single-stage design has 3 perturbed operating points with $v\text{-gaps}$ less than 0.3, while all $v\text{-gap}$ values of the two-stage design are above 0.3. Hence, the two-stage design exhibits stronger nonlinearity behaviour, which presents more difficulties to process control than the single-stage design. But, it would only become clear to what extent this difference affects the dynamic controllability once the result of optimization based on problem **P-5.2** is obtained.

Since the values of $v\text{-gap}$ could be either enlarged or narrowed depending upon the chosen values of input weights (W_e), it is desirable to find the values that actually minimize the worst $v\text{-gap}$ of the weighted plant. Since the values of W_e would affect the performance and robustness of the optimal controller designed, it is important that this dynamic performance must be within the specification (5-43) i.e. b_{opt} between 0.3 and 0.5.

The optimal weights, which minimize the $v\text{-gap}$ between nominal model and perturbed models of the single-stage and two-stage designs, are given by Eq. 5-45 and Eq. 5-46 respectively. In Table 5-5 and Table 5-6, the $v\text{-gap}$ analysis results of both designs under the optimal weights are presented. Also note that as shown in Table 5-6, the closed-loop performances under the optimal weights b_{opt} for both designs are almost similar (0.3018 and 0.3143) implying that their closed-loop performances are comparable at their respective nominal operating levels.

From Table 5-5, notice that under the optimal controller, the worst distance is unaltered but some distances are reduced i.e. P3 and P5 while other distances increase. For the single-stage design, there are 3 of the perturbed points which are guaranteed (v-gap values within b_{opt}) to be stabilized by the optimal controller i.e. *P3*, *P4* and *P6*. From Table 5-6, notice that none of the v-gap values under the optimal controller lies within the specified b_{opt} for the two-stage design. Therefore, this indicates that the two-stage design has stronger nonlinearity behaviour than the single-stage design. Thus from the linear control perspective, single-stage design has better controllability property than the two-stage design.

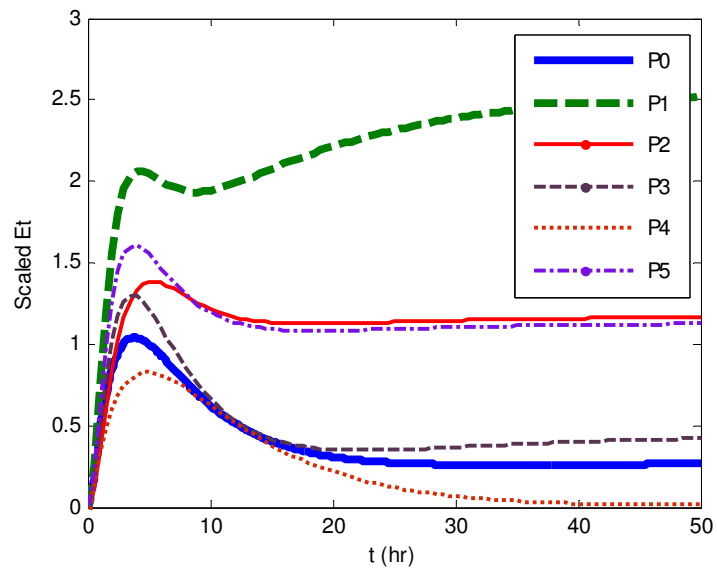


Figure 5-5: Open loop ethanol concentration (single-stage) subject to unit step change in F_0

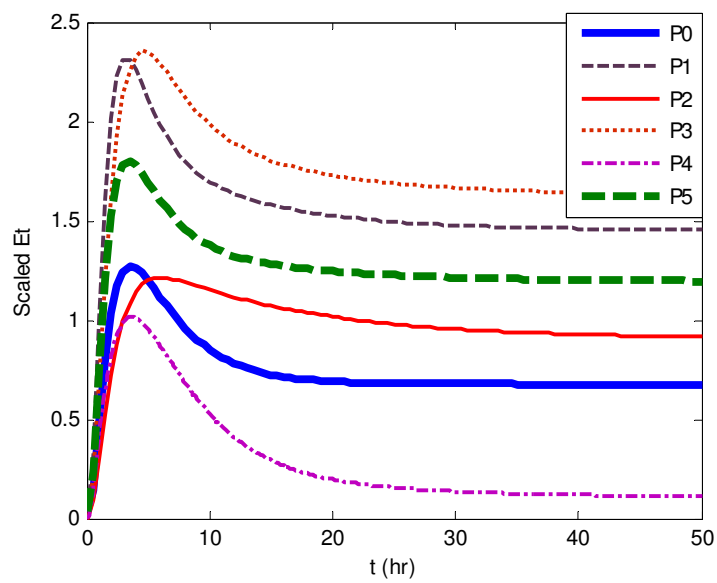


Figure 5-6: Open-loop ethanol concentration (two-stage design) a subject a unit step change in F_0

Table 5-5: The ν -gap for the single-stage design

Operating Level	Not Weighted	Weighted
P0	0	0
P1	1.000	1.000
P2	0.995	1.000
P3	0.357	0.270
P4	0.222	0.229
P5	0.498	0.470
P6	0.194	0.207
P7	0.936	0.940
P8	0.662	0.688

Table 5-6: The ν -gap for the two-stage design

Operating Level	Not Weighted	Weighted
P0	0	0
P1	0.678	1.000
P2	0.337	0.917
P3	0.385	0.804
P4	0.703	0.350
P5	0.325	0.584
P6	0.804	0.611
P7	0.891	0.719
P 8	0.962	0.852

Table 5-7: Plant optimal performance b_{opt}

b_{opt} for single-stage design		b_{opt} for two-stage design	
Not Weighted	Weighted	Not Weighted	Weighted
0.7120	0.3018	0.6745	0.3143

For the single-stage design an optimal robust controller can be designed to stabilize the three perturbed operating points with the v -gap less than that of b_{opt} (P3, P4 and P6). As for the two-stage design, all the values of v -gap are above that of $b_{opt} = 0.3143$. Hence this implies that it is more difficult to design a controller (based on nominal operating level) that is guaranteed to stabilize any of the perturbed operating conditions, or if any the closed-loop performance is probably not guaranteed to acceptable.

The optimal weight for the *single-stage design*:

$$W_{e,1} = \begin{bmatrix} \frac{-8.99s-1.19}{s(19.16s+1)} & 0 & 0 \\ 0 & \frac{5.30s+2.31}{s(10.16s+1)} & 0 \\ 0 & 0 & \frac{-17.52s-4.71}{s(20.53s+1)} \end{bmatrix} \quad 5-46$$

And the optimal weight for the *two-stage design*:

$$W_{e,2} = \begin{bmatrix} \frac{-11.44s-11.34}{s(22.68s+1)} & 0 & 0 \\ 0 & \frac{0.186s-0.37}{s(29.67s+1)} & 0 \\ 0 & 0 & \frac{-13.8s-1.65}{s(4.9s+1)} \end{bmatrix} \quad 5-47$$

To confirm this analysis, we perform a number of closed-loop simulations for both designs. Figure 5-7 shows the closed-loop performance (ethanol concentration) of the single-stage design at different perturbed operating points ($P1$, $P3$ and $P4$) based on linearized models. It can be seen that the optimal controller designed at the nominal operating point is not stable at the perturbed operating point $P1$. This is expected because the v -gap between the nominal and this perturbed levels $\delta(P_0W_e, P_1W_e) = 1.0$, which is much larger than that of $b_{opt} = 0.3018$.

But, the controller is able to perform well (stable) at perturbed operating points $P3$ and $P4$ since at these levels the v -gaps (0.27 and 0.229 respectively) are smaller than b_{opt} . Also as expected, the performances at these operating points ($P3$ and $P4$) are comparable to that of the nominal one.

Moreover, Figure 5-8 demonstrates the closed-loop performance for the two-stage design at the different perturbed operating points (P1, P3 and P4). Similar to the single-stage case, the controller is unable to stabilize the P1 level because the $v\text{-gap}$ value of this operating point (as shown in Table 5-6 is much larger than b_{opt} value of 0.3143. The controller designed at the nominal level is able to stabilize the other perturbed levels P3 and P4. However, the performance is as good as compared to the performance at the nominal operating point i.e. very sluggish.

Furthermore, by comparing Figure 5-7 and Figure 5-8 it can be seen that the single-stage design is more responsive than the two-stage i.e. shorter settling times when operating at P3 and P4.

Figure 5-9 shows the simulation result for the setpoint tracking (unit step change in ethanol concentration) based on the actual nonlinear model for the single-stage design. Interestingly, for the single-stage design, the controller designed at the nominal level is only unstable at P1 and P2 i.e. the controller can stabilize 6 other perturbed operating levels.

Figure 5-10 indicate the responses for the setpoint tracking of the two-stage design based on the actual nonlinear model. For the first 150 hrs (simulation time) most of the perturbed responses are stable and comparable with the response at $P0$. But many of the responses are unstable (exhibit slow drift) after 150 hrs where in fact the controller can stabilize only 4 perturbed levels i.e. $P3$, $P4$, $P6$ and $P7$. This is not surprising since the $v\text{-gap}$ values of two-stage design are all beyond the value of the specified b_{opt} .

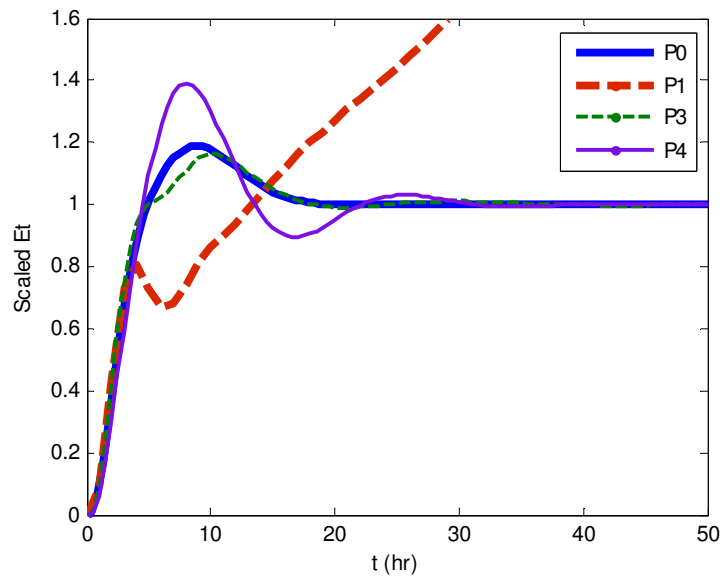


Figure 5-7: Setpoint tracking (ethanol) of single-stage under optimal feedback controller based on linearized models, $b_{opt} = 0.3018$

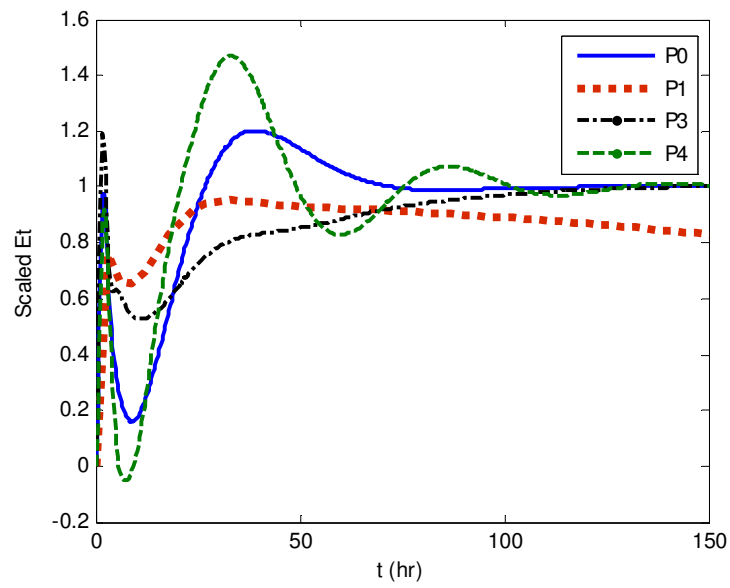


Figure 5-8: Setpoint tracking (ethanol) of two-stage under optimal feedback controller based on the linearized models, $b_{opt} = 0.3143$

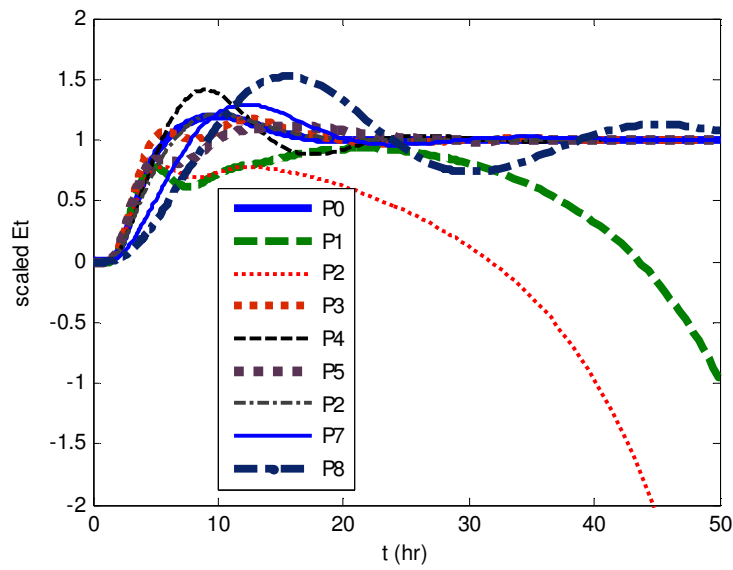


Figure 5-9: Setpoint tracking (ethanol) of single-stage based on nonlinear model

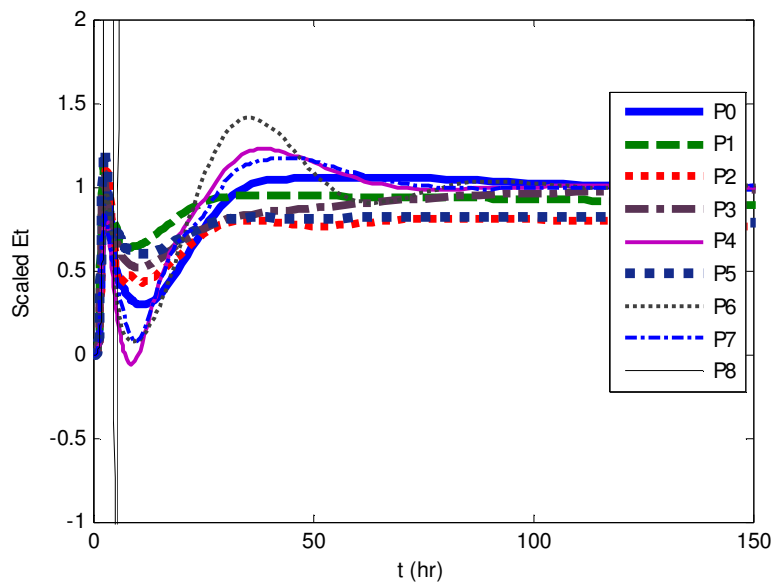


Figure 5-10: Setpoint tracking (ethanol) for two-stage design based on nonlinear model

5.10 Summary

Nonlinear modeling of a case study process called the two-stage continuous extractive (TSCE) alcoholic fermentation system is developed in this chapter. Then optimization based on the response surface methodology is performed to obtain the operating conditions, which give the *optimal trade-off* between yield and productivity of ethanol. It is found that the optimal trade-off values between yield and productivity for two-stage design are 82 % and 21 kg/m³.hr respectively. Hence, the two-stage and single-stage designs exhibit comparable steady-state performance in term of the optimal trade-off values between yield and productivity. However, two-stage design requires significantly smaller total bioreactor volume than that of single-stage design – two-stage design shows potential economic benefit.

Additionally, in this chapter a new framework for the dynamic controllability analysis which integrates the concepts of control relevant metric (*v-gap*), factorial design of experiment and multi-objective optimization is developed. While *v-gap* is used to quantify the nonlinearity or distance between the nominal (operating level) model and perturbed (operating level) model, the factorial design of experiment is used to generate the minimum number of perturbed operating levels required. For each perturbed operating level, a linearized model is obtained, and the distance between this perturbed model and the nominal model is quantified via *v-gap metric*. Then the weight values (W_e) are optimized in such a way to minimize the distances (not just the worst distance) – i.e. application of multi-objective optimization formulation.

The new dynamic controllability methodology is then used to analyze the dynamic controllability of the two-stage and single-stage designs. Result of the dynamic controllability analysis shows that, the two-stage design exhibits stronger nonlinearity than that of the single-stage design. Therefore, the analysis suggests that the two-stage design is more difficult to control than the single-stage design. However, it is important to note that this analysis is mainly from the controller algorithm point of view. It does not consider how the choice of the controlled variables will affect the process controllability. In other words, if we use similar controlled variables and manipulated variables and also adopt similar controller algorithm, then it would be easier to control the single-stage design than the two-stage design.

6 BASIC PARTIAL CONTROL DESIGN FOR TSCE ALCOHOLIC FERMENTATION SYSTEM

6.1 Introduction

It is desirable to have a simple and practical control structure design for the chemical and bio-chemical processes. In this regard, *partial control philosophy* can serve as a guiding principle for the engineers to design a simple control strategy, which only requires minimum number of sensors. However, as mentioned previously in Chapter 2 the key drawback to adopting partial control idea rests on its heavy reliance on process knowledge and engineering experience. In Chapter 3, we have described a new framework for implementing partial control idea which makes use of the concept of Principal Component Analysis (PCA) to identify the dominant variables.

Consequently, a methodology of complete partial control design has been developed and presented in Chapter 4. Therefore, in this chapter, we will demonstrate the use of the key results developed in Chapter 3 (and part of Chapter 4) on the design of basic partial control strategy for the TSCE alcoholic fermentation system, which has been described previously in Chapter 5. The complete design of partial control strategy based on the methodology described in Chapter 4 will be explored in the next Chapter 7.

Note that, the result of the basic partial control design for the TSCE alcoholic fermentation system has been published in Journal of Chemical Product and Process Modeling (Nandong, Samyudia and Tade 2010).

6.2 Basic Partial Control Structure Design

6.2.1 Step 1- Performance Measures Specification

Three implicit performance measures are identified as: (1) ethanol yield (*Yield*), (2) substrate conversion (*Conv*), (3) and ethanol productivity (*Prod*). The overall control

objective is to maintain *Yield*, *Conv* and *Prod* around their optimal values, which are 81%, 90% and 21 kg/m³.hr (i.e. optimal results from Chapter 5) respectively, such that, the variations or losses in performance measures in the face of disturbance occurrence are acceptable. Let the maximum acceptable variations in performance measures are:

$$\Delta\Phi_{\max} = \begin{bmatrix} 1.0\% \\ 1.0\% \\ 1.0\% \end{bmatrix} \quad 6-1$$

Where:

$$\Phi = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} \text{Yield} \\ \text{Conv} \\ \text{Prod} \end{bmatrix} \quad 6-2$$

6.2.2 Step 2- Design of Experiment – Data Generation

The inputs selected for the factorial design of experiment are (1) fresh substrate flowrate F_o , (2) inlet substrate concentration S_o , (3) cell recycle ratio R , and (4) flash liquid recycle ratio r . Table 6-1 shows the coded and real values used for the factorial design of experiment. These inputs are chosen on the basis of their known strong influence on the system (i.e. based on the process knowledge). In the absence of prior knowledge, it is helpful in selecting which inputs are to be used in design of experiment by conducting a preliminary dynamic simulation study (open-loop) on the system of interest. The nominal values of F_o , S_o , R and r are selected as 100m³/hr, 120kg/m³, 0.225 and 0.27, respectively. These values correspond to the optimal trade-off between *Yield* and *Prod* (Nandong, Samyudia and Tadé 2006).

The magnitude of input perturbation applied is $\pm 20\%$ of their nominal values. Based on the factorial design of experiment, there is $2^4 = 16$ number of experimental runs i.e. this corresponds to 16 perturbed operating levels. In total there are 17 runs including the one at the nominal operating level. Note that, it is important that the size of the input perturbation to be large enough as to result in some outliers in the plant data. To get a good idea of how large the input size should be, one can perform a preliminary dynamic simulation study on the process of interest.

Table 6-1: Real and coded values used for factorial design

Input	Level (-1)	Level (0)	Level (+1)
F_o (m ³ /hr)	80	100	120
S_o (kg/m ³)	96	120	144
R (-)	0.180	0.225	0.270
r (-)	0.216	0.270	0.324

Table 6-2: Variables and performance measures forming dataset X

Output Variables	Input Variables
Bioreactor substrate concentration: S_1, S_2	Fresh substrate flowrate: F_o
Bioreactor ethanol concentration: Et_1, Et_2	Fresh substrate concentration: S_o
Bioreactor viable cell concentration: Xv_1, Xv_2	Cell recycling stream: R
Bioreactor temperature: T_1, T_2	Flash recycling stream: r
Bioreactor liquid level: L_1, L_2	
Performance Measures	Process Parameters
Ethanol Yield: <i>Yield</i>	Rate of growth: rx_1, rx_2
Substrate Conversion: <i>Conv</i>	Rate of substrate consumption: rs_1, rs_2
Productivity: <i>Prod</i>	Rate of ethanol formation: rp_1, rp_2

Remark 6.1:

The reason to include the input variables in the dataset X in the identification of dominant variables is that to enable us to analyze whether the input variables have strong impact on the performance measure (see Chapter 3, significances of Closeness Index). If the input u_i has a strong impact on the performance measure (i.e. it is a dominant variable), then it should not be used as a manipulated variable for controlling y_j . However, if input u_i and output variable y_j are correlated and both are dominant variables for the performance measure of interest, and then in this case u_i can be used as the manipulated variable for controlling the y_j .

□

6.2.3 Step 3- Identification of Dominant Variables

Successive dataset reductions (as described in Chapter 3, Section 3.4.2) are performed using PCA on the dataset X , which consists of 23 elements (4 inputs, 10 outputs, 6 process parameters and 3 performance measures) and 17 observations. Thus, the size of the dataset X is 17 by 23 i.e. there are 17 observations and 23 variables including performance measures and process parameters. Table 6-2 shows the variables, parameters and performance measures that form the dataset X .

Remark 6.2:

Process parameters such as the rate of growth can be considered in the analysis of dominant variables assuming that they are measurable e.g. by mean of soft-sensor. Otherwise, do not include the process parameters in the dataset X . Here it is assumed that the rate of growth is measurable.

□

With regard to the process parameter, it is important to distinguish this term from the equipment design parameters, such as reactor volume, heat exchanger surface area, etc. In this thesis, the term “process parameter” refers to model parameter which is a function of process variables e.g. growth rate which depends on substrate concentration and temperature. On the other hand, the equipment parameter is normally not a function of process variables i.e. reactor volume will not change with reactor temperature.

Figure 6-1 shows the 2D-plot of PCA for the original dataset X . Note that, the sum of variances of PC-1 and PC-2 is more than 70%, thus implies that the 2D-plot of PCA is sufficient i.e. no need for the 3D-plot. From the enlarged plot (not shown here), one can see that all of the 3 performance measures are in the sub-dataset X_1 . Upon inspection, there are 9 variables in X_1 which may have some correlations with the performance measures, which are S_o , Xv_1 , Xv_2 , S_1 , S_2 , rs_2 , rp_2 , rx_2 and R .

Also, there are *few outliers* in the 3rd quadrant, thus showing that X_I fulfils all of the 3 dominant variable (DV) criteria. In other words, the dominant variables could be among these 9 variables. Now, we apply another PCA on the sub-dataset X_I in order to further reduce the number of variables.

Figure 6-2 shows the PCA plot for X_1 sub-dataset. From the plot, one can now identify that all of the performance measures are in X_{12} sub-dataset. The plot indicates that *Yield* and *Conv* are positively correlated with each other, but are negatively correlated with the *Prod*. This is consistent with the previous report in (Nandong et al. 2006, Costa et al. 2001) where *Yield* and *Conv* are having the opposite trend to that of *Prod*. Based on the enlarged plot (not shown), the variables that are in X_{12} are R , rx_2 , S_I and S_2 . Thus, we have reduced the number of variables from 9 to 4 variables.

Notice that, the sum of variances of PC-1 and PC-2 is 85% which is equal to the *threshold* value v_{cric} . Thus, this shows that the critical dominant variable condition has been reached, and we can stop at this second level of dataset reduction. Furthermore, notice that there is an outlier (at observation #6) in the sub-dataset, thus all DV criteria are fulfilled.

Because all DV criteria are completely fulfilled up to this dataset reduction level, hence it can be concluded that these 4 variables are the dominant variables for *Yield*, *Conv* and *Prod*. In other words, if the variables are kept constant, the steady-state variations or offsets of these performance measures will be guaranteed to be small in the face of external disturbance occurrence.

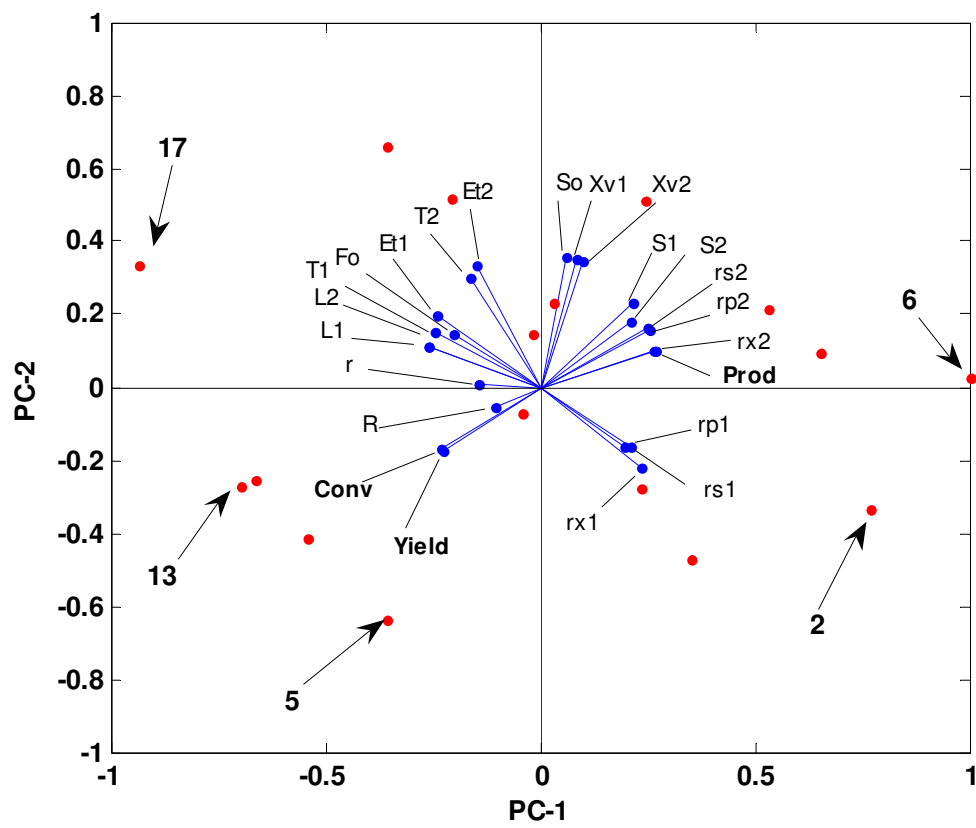


Figure 6-1: PCA plot for dataset X: sum of variances PC1 + PC2 = 80%

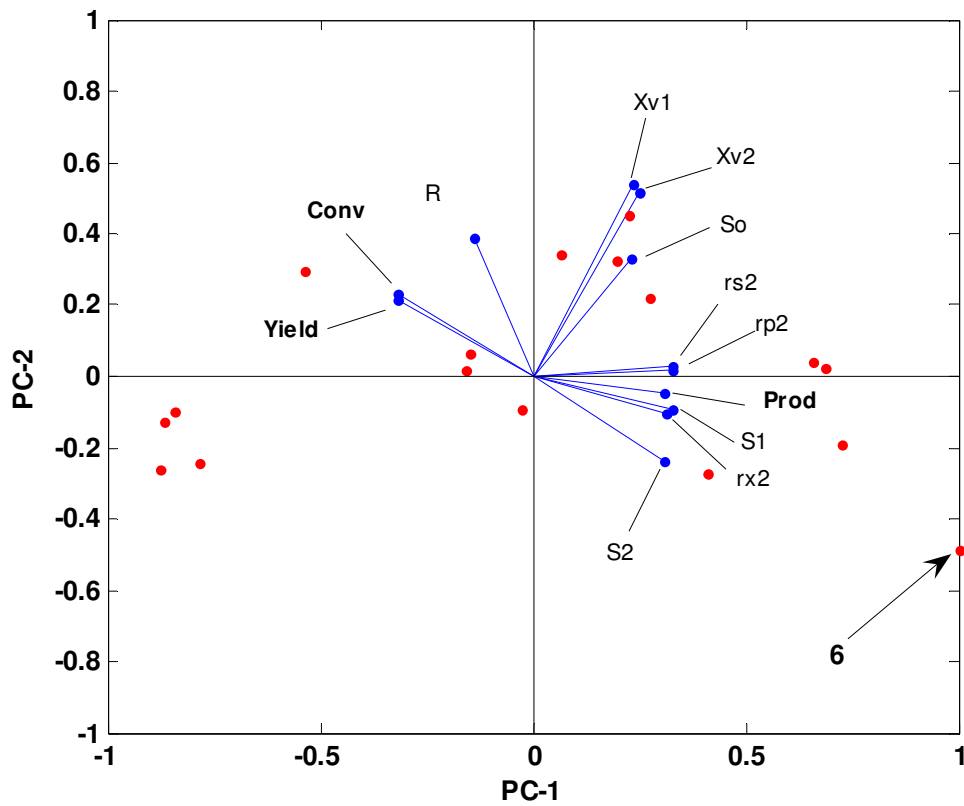


Figure 6-2: PCA plot for X_1 sub-dataset: variances of PC1 + PC2 = 85%

Thus, it can be concluded that the mapping from the set of performance measures onto the set of dominant variables results in:

$$\begin{Bmatrix} Yield \\ Conv \\ Prod \end{Bmatrix} \rightarrow \begin{Bmatrix} S_1 \\ S_2 \\ rx_2 \\ R \end{Bmatrix}$$

Interestingly, in this case all of the performance measures have similar dominant variables. Thus, this implies strong correlation among the performance measures. Also notice that, R is one of the dominant variables. Because this input correlates with other dominant variables (which are output variables), therefore R can be chosen as a manipulated variable to control one of the dominant (output) variables.

6.2.4 Step 4: Control Structure Design Decisions

One of the key tasks in Step 4 is to select which dominant variables to be controlled i.e. as the primary controlled variables. To facilitate the accomplishment of this task, we can adopt the concept of closeness index described in Chapter 3 (Section 3.4.3). Here, we will definitely control the strongest dominant variable i.e. the one with the smallest value of closeness index.

Step 4.1: Selection of Primary Controlled Variables

Note that, we focus on the 3 output variables in the dominant variable set where the input variable (R) is left as a possible manipulated variable. Now let:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} S_2 \\ S_1 \\ rx_2 \end{bmatrix} \quad 6-3$$

The value of the closeness index for each dominant variable in the direction of each performance measure is shown in Table 6-3. Notice that, the closeness index of S_2 for each performance measure is less than 0.09 i.e. $\delta_{1j} < 0.09$ for $j = 1, 2, 3$. All the values of closeness index of S_2 are the smallest as compared to the other dominant variables, with the exception of closeness index of rx_2 on *Prod* ($\delta_{33} = 0.051$). This indicates that S_2 is the strongest dominant variable which strongly influences all performance measures – it fulfils the first *Primary Controlled Variable criteria* i.e. PCV criteria 1 (Chapter 4, Section 4.4.4). However, in particular the influence of rx_2 is stronger than the influence of S_2 on the *Prod* i.e. $\delta_{33} < \delta_{13}$.

Consequently, in this case we decide to control rx_2 as well as S_2 where the former is expected to have more tight (indirect) control on *Prod*, and the latter to have tight control on *Yield* and *Conv*. Note that, the selection of S_2 as one of the primary controlled variable is justified because it fulfils the PCV criteria 1 to 3 (see Chapter 4, Section 4.4.4). Meanwhile, the selection of rx_2 as another controlled variable is considered on the basis that this will lead to more tight control on *Prod*. We will further investigate whether this is truly necessary in the next Chapter 8.

Table 6-3: Values of closeness index

Dominant variable	Yield (ϕ_1)	Conv (ϕ_2)	Prod (ϕ_3)
y_1 (S_2)	$\delta_{11} = 0.002$	$\delta_{12} = 0.019$	$\delta_{13} = 0.083$
y_2 (S_1)	$\delta_{21} = 0.163$	$\delta_{22} = 0.193$	$\delta_{23} = 0.084$
y_3 (rx_2)	$\delta_{31} = 0.167$	$\delta_{32} = 0.194$	$\delta_{33} = 0.051$

Based on the analysis via closeness index, the set of selected primary controlled variables ($Y_{CV,P}$) is given as follows:

$$Y_{CV,P} = \{S_2, rx_2\} \quad 6-4$$

Remark 6.3:

Notice that, if S_1 is controlled rather than S_2 , then we can achieve faster dynamic response on the assumption that the point of entry for the disturbance is closer to S_1 than to S_2 i.e. disturbance enter through bioreactor 1. But this assumption is not necessarily valid for the case with recycle system – i.e. two recycle-loops as in the case study process. In practise, there could be several sources of disturbances which enter from various points. In a serial system with recycle structure, most of the disturbance effect will end up in the last system. If the control is imposed on an upstream system, then this only absorbs the effect of disturbance in that system only. However, the effect of disturbance on the down stream system will only be partially absorbed. The presence of recycle structure will eventually propagate this unabsorbed effect back to the upstream system. Thus, it would be better to control the downstream system because this leads to the removal of most disturbances effect.

□

Step 4.2: Selection of Manipulated Variables

The next task is to select the manipulated variables U_{MV} from the set of available input variables U . Note that, in this study the selection of manipulated variables is not as difficult as the selection of controlled variables. The reason is that, we have only a small

number of input variables as compared to output variables i.e. 6 inputs and 16 outputs. Therefore, in this case study we simply select the manipulated variables based on process knowledge obtained via preliminary simulation study and literature i.e. rigorous technique is not applied. However, in practice it is advisable to employ some of the quantitative tools such as the Morari Resiliency Index (MRI) to help in the selection of manipulated variables especially if the number of input variables is large.

In this case study, there are six potential manipulated variables as:

$$U = \{F_1, F_2, r, R, F_o, F_v\} \quad 6-5$$

Owing to its strong influence on the selected primary controlled variables (Step 4.1), the cell recycle ratio (R) is selected as one of the manipulated variables. Another input chosen as manipulated variable is F_o due to its direct influence on the substrate concentration. Thus, the set of manipulated variables (U_{MV}) is given by:

$$U_{MV} = \{R, F_o\} \quad 6-6$$

Step 4.3: Determination of Controller Pairings

Using the RGA analysis, the favourable pairings which minimize the control-loop interaction are found to be R - S_2 and F_o - rx_2 . Next, linear PI controllers are designed and used for both control loops. In this study, the PI parameter tuning is not optimized. We adopt simple tuning procedure based on the Ziegler-Nichols for each loop followed by detuning to reduce the controller aggressiveness. The performance of the multi-loop SISO control system is tested against a step change in the fresh substrate concentration (S_o) with magnitude equals to 30 kg/m^3 i.e. 25% of the nominal value of disturbance.

6.3 Dynamic Simulation of Basic Partial Control Strategy

Figure 6-3 and Figure 6-4 show the closed-loop responses of S_1 , S_2 and rx_2 when subject to step change in S_o . Notice that, the responses of S_1 and S_2 exhibit similar shape implying closed correlation between them i.e. as anticipated from the previous PCA analysis. Although the disturbance magnitude is severe, the system remains stable. But, the responses of controlled variables to step down in S_o is significantly slower than that

to step up in S_o . This shows that the system is highly nonlinear - recall the result of dynamic controllability analysis in Chapter 5.

Furthermore, notice that the responses of L_1 and L_2 exhibit similar trend which show that these two variables are also dynamically coupled (as predicted by the PCA-based analysis previously). Figure 6-4 displays that the magnitude of peak values for L_1 and L_2 are quite large i.e. about ± 1.0 m in bioreactor 1. This is not desirable because it means that we cannot operate close to the maximum bioreactor volume. It is usually desirable to operate close to the maximum volume of reactor in order to achieve improved economic performance.

Figure 6-5 shows the closed-loop responses of *Yield*, *Conv* and *Prod* subject to the S_o step changes. To evaluate the effectiveness of this partial control structure, one can look at the steady-state offsets in *Yield*, *Conv* and *Prod* – i.e. if indeed our choice of controlled variables is the dominant variables, then the offsets must be small.

The steady-state offsets in *Yield*, *Conv* and *Prod* in this case is less than 0.1%, thus showing the effectiveness of the partial control strategy in term of reducing the steady-state offsets. Interestingly, the variations in the performance measures are much smaller than the specified value which is 1.0%.

The small offsets in performance measures (which are implicit functions of process variables) confirm that the selected controlled variables are indeed having strong correlation (influence) with them. In turn, this result confirms that they are the dominant variables for the performance measures – validates the application of the PCA-based technique.

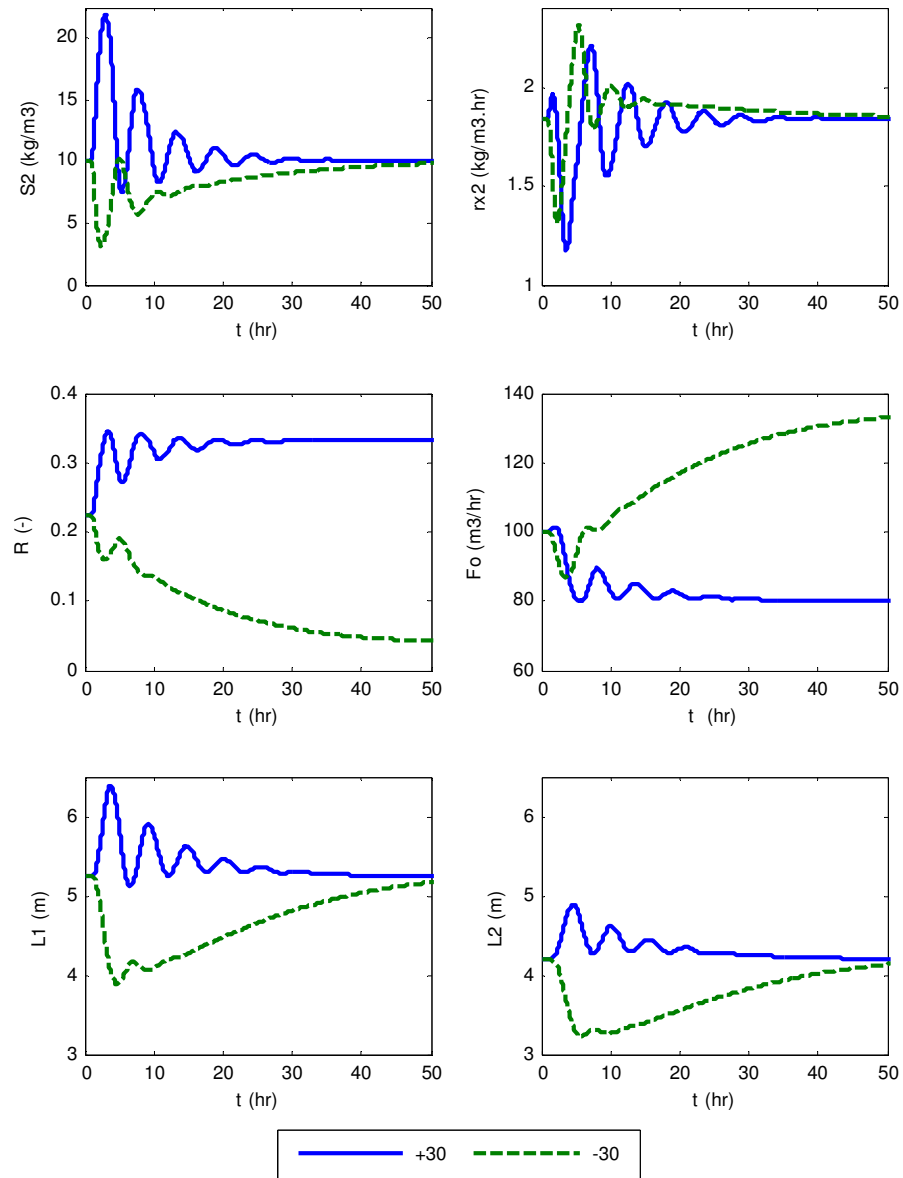


Figure 6-3: Closed-loop responses to step change in S_0 by $\pm 30 \text{ kg/m}^3$ for S_2 , rx_2 , R , F_0 , L_1 and L_2

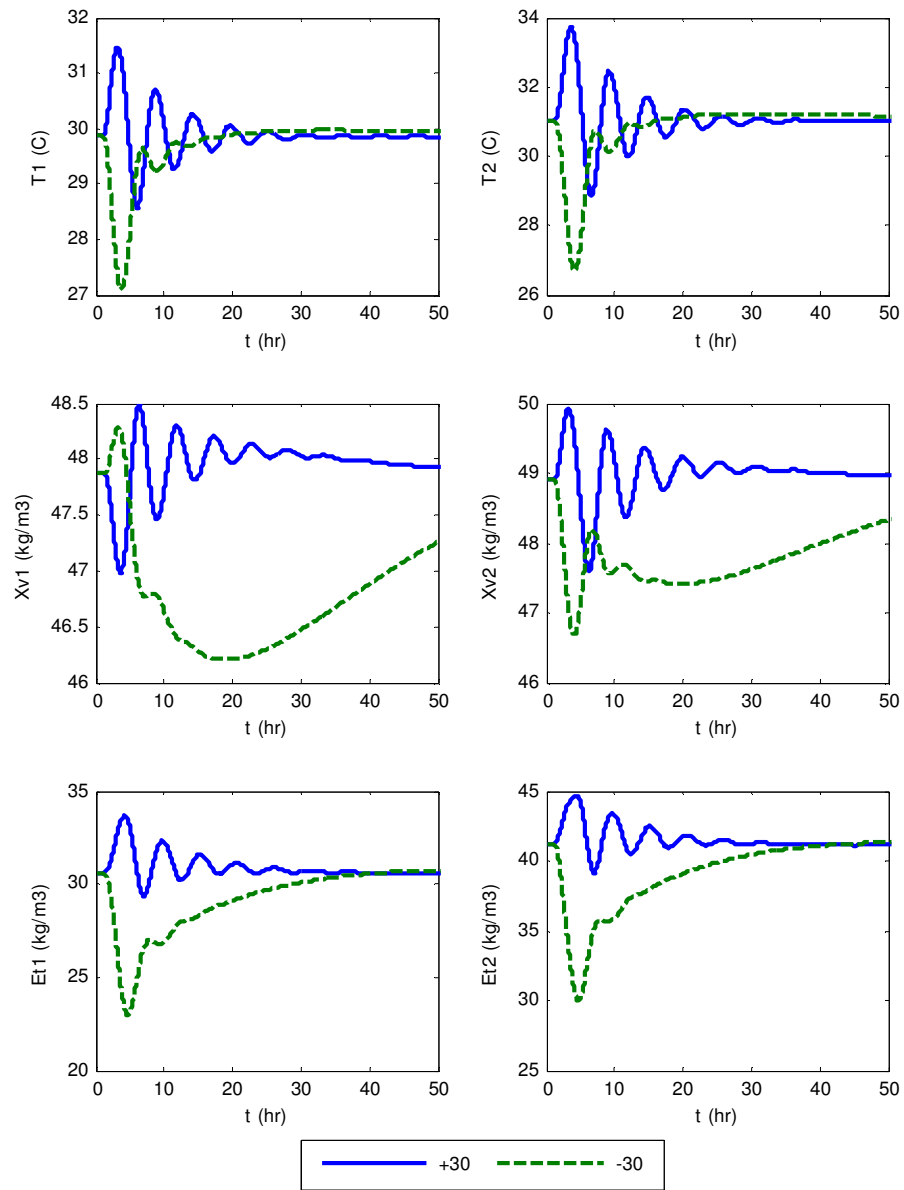


Figure 6-4: Closed-loop responses to step change in S_o by $\pm 30 \text{ kg/m}^3$ for T_1 , T_2 , X_{v1} , X_{v2} , E_{t1} and E_{t2}

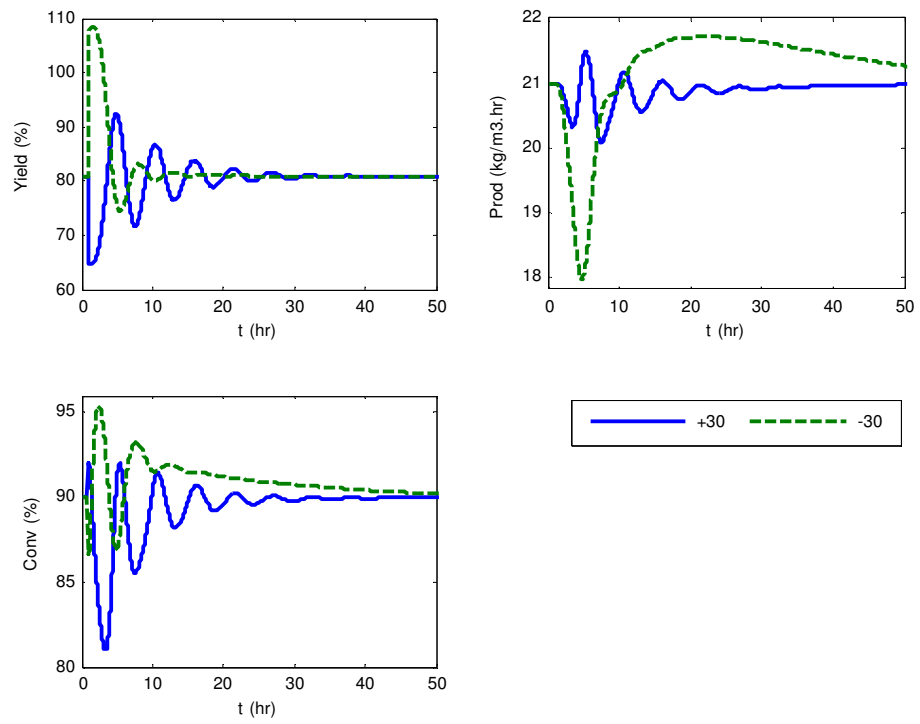


Figure 6-5: Yield, Conv and Prod responses to step change in S_o : $\pm 30 \text{ kg/m}^3$

Table 6-4 shows the peak values of temperatures and ethanol concentrations during their transient responses. It is important to note the peak values of these variables because the values that are too high can damage the yeast cells, hence leading to slow decay of productivity and yield. In this case, it is desirable to keep the temperature below 33°C and the ethanol concentration at around 40kg/m³ i.e. industrial practice as reported in Costa et al (2001). Table 6-4 clearly shows that the peak value of T_2 already violates the maximum threshold value of 33°C. The other variables seem to have reasonable peak values i.e. below threshold for T_1 Et_1 and quite close to threshold value for Et_2 . In this case, the most critical variable is T_2 (temperature in bioreactor 2) because when the temperature exceeds 33°C, the yeast cells activity start to go down drastically – leading to reduced yield and productivity.

Notice that, the peak excursion in ethanol concentration Et_2 is about 10% of the industrial practice. In this case, this is quite acceptable because the threshold concentration of ethanol for *S. cerevisiae* beyond which growth rate is completely retarded is about 12% w/v. Thus, in this case the concentration of ethanol 40 kg/m³ (approximately 4% w/v) is still far from this threshold value.

It should be remembered that, the dynamic responses of *Yield*, *Conv* and *Prod* tend to follow the dynamic responses of S_2 and rx_2 , which in other words tend to follow their corresponding dominant variables responses (Figure 6-3 and Figure 6-5).

In contrast, large variations in L_1 , L_2 , Et_1 , Et_2 , Xv_1 and Xv_2 during the transient responses seem to have very little effects on the transient responses of performance measures. This is not surprising because these variables are not the dominant variables for the performance measures.

Table 6-4: Peak values of output (constraint) variables during their transient responses

	T1 (°C)	T2 (°C)	Et1 (kg/m³)	Et2 (kg/m³)
Peak	31.5	33.7	33.7	44.7

There are few weaknesses of the current basic partial control strategy which still need to be addressed in real practice as:

- 1) Long recovery of performance measures especially the productivity (*Prod*) i.e. probably due to sluggish response of primary controlled variable, rx_2 .
- 2) Constraint violation by T_2 during transient response can cause damage to yeast cells (see Table 6-4) i.e. T_2 must be below 33°C.
- 3) Unacceptably large variations or fluctuations in L_1 and L_2 during transient responses, which can lead to inefficient use of reactor volume i.e. prevents the operation of bioreactors close to their maximum values.

6.4 Discussion on Basic Partial Control Strategy

It is important to note that the partial control strategy developed for the extractive fermentation system in this case study is only a basic partial control design. Thus, its performance can be further improved by applying some of the PID enhancement techniques such as, cascade and ratio control strategies. Furthermore, to make the partial control design fully functional for large-scale plant, we generally need to add inventory control as well e.g. level control.

Overall, although the partial control strategy adopted in this case study is very simple (i.e. we only control 2 out of 16 output variables), its steady-state performance is more than acceptable because the variation in performance measures is much less than the specified maximum value. Additionally, it is robust in the face of a large change in the inlet substrate concentration S_o – i.e. it remains stable.

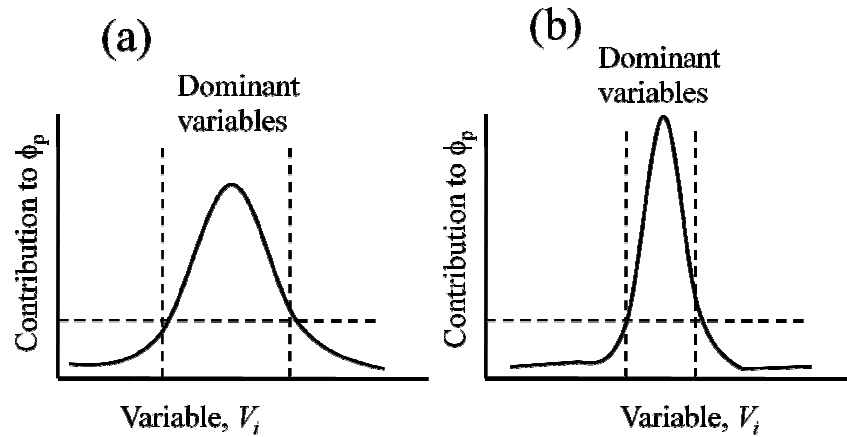


Figure 6-6: Illustration of two different plant scenarios: (a) large number of dominant variables, (b) small number of dominant variables

Figure 6-6 illustrates two different plant design scenarios corresponding to low and high values of v_{cric} . Low value of v_{cric} generally implies a large number of dominant variables (Figure 6-6a) for a given performance measure ϕ_p , which means that the contributions of the variables to ϕ_p are more widely distributed. In contrast, high value of v_{cric} normally leads to small number of dominant variables (Figure 6-6b) but each of the variables has very large contribution relative to other non-dominant variables.

For partial control, it is desirable to have small number of dominant variables because this leads to less controlled variables, and in turn yields less complex control strategy. However, it is important to bear in mind that, the number of dominant variables is strongly related to the flowsheet design – i.e. different design has different dominant variables and distribution of their contributions to a given performance measure.

Another important point to note is that, the algorithm for implementing the PCA-based technique proposed so far is based on a system which is open-loop stable. Thus, it is not directly applicable to *non-equilibrium systems* such as batch and open-loop unstable processes. However, the PCA-based technique can still be applied to these systems but the algorithm for implementing the technique need to be modified.

6.5 Summary

In this chapter, we have demonstrated the use of the so-called *PCA-based technique* within the context of a new theoretical framework of partial control developed in Chapter 3. The PCA-based technique (i.e. data-oriented approach) is used to identify the dominant variables corresponding to 3 overall performance measures (i.e. *Yield*, *Prod* and *Conv*) for the TSCE alcoholic fermentation system – case study. All of these performance measures are *implicit functions* of process variables, and as such the dominant variables cannot be straightforwardly identified based on process experience and knowledge i.e. without any systematic tool it is difficult to identify the dominant variables.

Application of the PCA-based technique shows that there are 4 dominant variables (S_1 , S_2 , rx_2 and R) that correspond to the specified performance measures where 3 of them are output variables and 1 is input variable. Using the closeness index (CI) analysis, it is determined that S_2 has the strongest impact on the performance measures, with the exception of its impact on *Prod* i.e. where rx_2 has stronger influence on *Prod* than S_2 . Based on the CI analysis, S_2 is adopted as one of the controlled variables for its tight influence on *Yield* and *Conv*, and rx_2 is adopted as another controlled variable on the basis of its tight influence on *Prod*.

Simulation study shows that the basic partial control strategy is able to achieve the steady-state performance where the variations in performance measures are less than the specified bound, which is 1% and where the actual variations are less than 0.1%. Thus, this confirms that the controlled variables (S_2 and rx_2) are indeed the dominant variables corresponding to the specified performance measures. In turn, this result validates the effectiveness of the PCA-based technique in the identification of dominant variables.

However, during the transient phase, the bioreactor 2 temperature (T_2) violates the maximum allowable limit which is 33°C. In practice, this is not desirable because temperature excursion above 33°C will dramatically reduce the yeast performance. Additionally, the fluctuations of liquid levels in both bioreactors are quite high, which means that we cannot operate close to the maximum bioreactor volume – hence, tends to cause lower economic performance.

It is important to remember that the basic partial control strategy discussed in this chapter only accounts for the overall performance objectives, and not the other types of

control objectives, namely the inventory and constraint control objectives. Thus, although the strategy achieves the overall performance objectives, unfortunately the other control objectives are not met. Despite these limitations, the control strategy is robust enough against the large disturbance occurrence i.e. large change in S_o . In the next Chapter 7, we will address how to incorporate the inventory and constraint control objectives into the design of partial control strategy.

7 COMPLETE PARTIAL CONTROL DESIGN FOR TSCE ALCOHOLIC FERMENTATION SYSTEM

7.1 Introduction

In Chapter 6, we have demonstrated the application of PCA-based technique to basic partial control design for TSCE alcoholic fermentation process. Interestingly, the PCA-based technique has been shown to be an effective tool in the identification of dominant variables which is otherwise, an intriguing task to perform if one relies solely on engineering experiences and process knowledge. The main reason for this complication is due to the highly interactive nature of the process variables.

Recalling the basic partial control design in Chapter 6, one realizes that the basic partial control design is quite insufficient from the plantwide control perspective due to the absence of inventory control. Furthermore, in the basic partial control design the constraints that relate to the process have not been carefully addressed. In other words, the basic design only focuses on the overall plant performance measures which are the maintenance of optimal trade-off between yield and productivity.

Although the basic partial control structure previously designed in Chapter 6 shows a good steady-state performance (i.e. very small variations in the key performance measures), its performance remains unsatisfactory because of:

- a) Large fluctuation of liquid levels in both bioreactors.
- b) High peak values of temperature and ethanol concentration in bioreactor 2.
- c) Slow recovery of the performance measures.

Thus, further improvements are required in terms of:

- a) Faster recovery of the performance measures.
- b) Lower peak values of temperatures and ethanol concentrations in both bioreactors.
- c) Lower fluctuation of liquid levels.

Addressing the last two objectives requires us to incorporate inventory and constraint control objectives into the basic partial control structure design. In this chapter, we will demonstrate how the complete methodology of partial control design

proposed in Chapter 4 can be applied to incorporating the inventory and constraint control objectives into the basic partial control design – known as the complete partial control design. Moreover, various strategies to enhance the dynamic performance of the complete partial control design will also be discussed in this chapter. Note that, part of this chapter is presented in DYCOPS 2010 (Nandong, Samyudia and Tade 2010).

7.2 Partial Control – Plantwide Design

7.2.1 Determination of Controlled Variables for Inventory Control

Inventory control is one the most important (and basic) aspects in a plantwide control design. The basic aim of inventory control is to ensure that there is no material accumulation within the system. For the two-stage continuous extractive (TSCE) alcoholic fermentation system described in Chapter 5, the variables which are within the inventory control group are the holdup liquid levels in the two bioreactors i.e. L_1 and L_2 . It is important to note that the holdup liquid levels in the vacuum-flash vessel and treatment tank are ignored on the basis that the dynamics of these two units are negligible as compared to the dynamics of the bioreactors. In other words, the liquid levels in the bioreactors are the main focus of inventory control.

An important question, is it necessary to control the liquid levels (L_1 and L_2) in both bioreactors? If L_1 and L_2 are strongly coupled or interacted with each other, then probably it is sufficient to control only one of them. Therefore, to answer this question we can apply the PCA-based technique described in Chapter 3 in order to find out whether they are strongly coupled or not.

Figure 7-1 shows the PCA plot for the sub-dataset X_2 containing L_1 and L_2 . Clearly, it can be seen from the figure that L_1 and L_2 are very closely correlated with each other (see quadrant 3). This suggests that it is only necessary to control either one of the liquid level in order to achieve the inventory control objective. In this case, we will evaluate two control structures namely CS1 which adopts L_1 as controlled variable (CV) and CS2 which uses L_2 as CV for the inventory control i.e.:

$$\text{Inventory control variable} \begin{cases} L_1 \text{ as CV for CS1} \\ L_2 \text{ as CV for CS2} \end{cases}$$

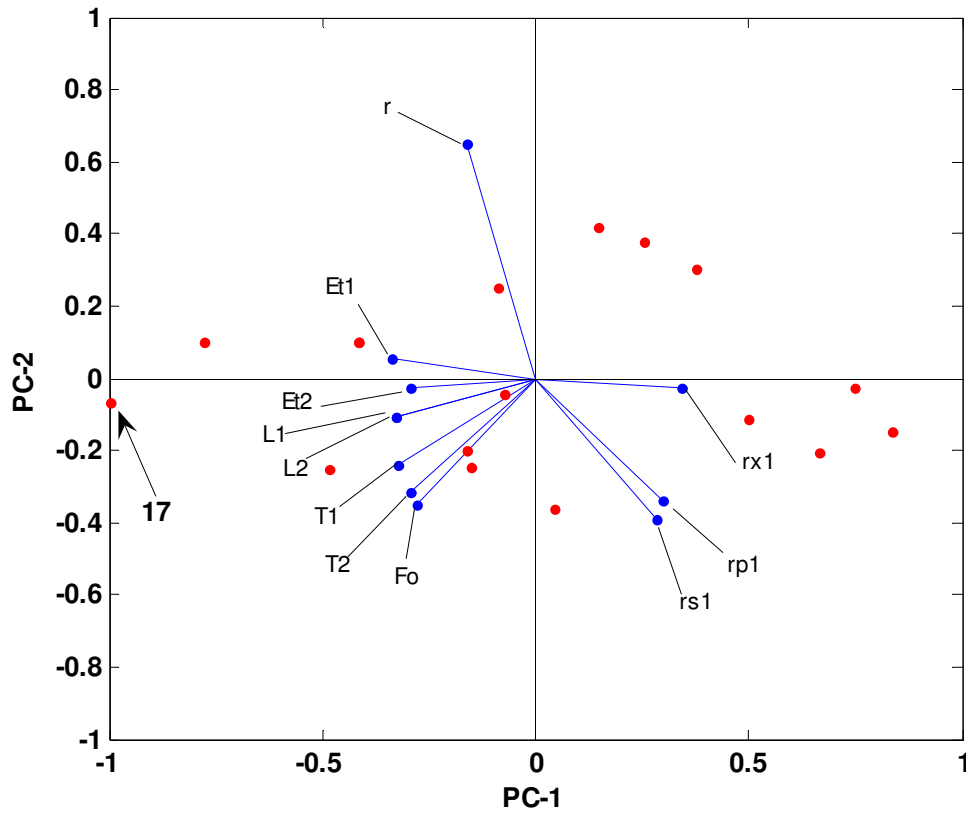


Figure 7-1: PCA plot for sub-dataset X_2

Remark 7.1:

Note that, the decision to control either L_1 or L_2 and not both is due to the fact these two inventory variables are strongly correlated. It is important to bear in mind that this decision is made on the assumption that the key (or majority of disturbances) enter through the first bioreactor. On the other hand, if the key disturbance enters through the second bioreactor, then it is better to control L_2 rather than L_1 because this would lead to maximum disturbance rejection. Furthermore, if the outlet flows from the bioreactors are controlled by pumps (i.e. integrating process) rather than by valves (self-regulating process), then we must control both liquid levels. In this case study, both outlet flows are controlled by valves and the main disturbance (fresh substrate concentration S_o) enters through the first bioreactor. Thus control of only one of the variables is sufficient.

□

7.2.2 Determination of Controlled Variables for Constraint Control

In order to determine the variables for constraint control, we need to adopt the process knowledge about the system i.e. there is no substitute to good process knowledge in the identification of process constraints. In this case study, we need to know what factors are limiting the performance of the yeast. Two important factors that need to be considered in the constraint control are (1) bioreactor temperature, and (2) ethanol concentration in the bioreactor.

For the optimum yeast activity, the temperature should be within the range of 28°C to 33°C. The upper limit which is 33°C should not be violated otherwise, the yeast activity will be seriously degraded i.e. the growth and product formation rates will be seriously retarded. Thus, bioreactor temperatures (i.e. T_1 and T_2) should be considered in the constraint control.

Another factor that needs to be addressed is the ethanol concentrations in the bioreactors. Based on industrial practice, the ethanol concentration in the last bioreactor (i.e. normally 4 bioreactors in series are used in industry) is maintained at about 40 kg/m³. When the ethanol concentration is too high above 40 kg/m³, then the inhibitory effect of the ethanol becomes more serious, which in turn can seriously slow down the growth and product formation rates. Thus, the productivity and yield of ethanol are greatly reduced at a very high ethanol concentration near a threshold value $C_{E,max}$. Obviously, from this perspective the concentrations of ethanol in both bioreactors should also be considered in the constraint control i.e.:

$$\text{Constraints} \begin{cases} \text{Bioreactor temperature} < 33^\circ\text{C} \\ \text{Ethanol concentration} < C_{E,max} \end{cases}$$

Overall we have 4 candidates for the controlled variables in the constraint control, which are T_1 , T_2 , Et_1 and Et_2 . Note that, we have only 6 potential manipulated variables, where 2 are already used in the primary control and 1 is used in the inventory control. Therefore, we are left with only 3 manipulated variables which mean that we cannot afford to control all of the 4 variables. As a result, we need to do evaluation in order to determine which of the candidates are to be controlled. Also, we need to know the sufficient number of controlled variables relating to the constraint control objectives.

Again we use the PCA-based analysis to find out how strong are the correlations among these 4 variables. Referring to Figure 7-1, we can see that T_1 , T_2 and Et_2 are strongly correlated with each other. Also, these three variables are correlated with L_1 and L_2 but to a lesser extent of course. This suggests that by controlling L_1 or L_2 , this will indirectly control T_1 , T_2 , and Et_2 . However, since the correlation is not sufficiently strong between $\{L_1, L_2\}$ and $\{T_1, T_2, Et_2\}$, there is no guarantee that the variations in $\{T_1, T_2, Et_2\}$ will be acceptable. As a result, we need to control at least one of the candidate variables i.e. either T_1 or T_2 or Et_2 in order to ensure the variations in $\{T_1, T_2, Et_2\}$ will be acceptable.

Notice that from Figure 7-1, Et_1 occupies quadrant 2 which means that it is not strongly correlated with T_2 . However, we can choose not to control Et_1 on the basis that its nominal operating value is lower than that of Et_2 i.e. 30.5 kg/m^3 and 40.5 kg/m^3 , respectively. Consequently, this means that we can allow high variability in Et_1 but not in Et_2 .

Our analysis so far has suggested that we should choose T_2 as a controlled variable to achieve the constraint control objectives for two reasons:

- 1) T_2 nominal operating value is larger than that of T_1 i.e. 31°C and 28.8°C , respectively. Hence, if disturbance occurs, it is more likely that T_2 will increase (overshoot) above 33°C than T_1 .
- 2) It is easier and cheaper to measure the temperature than to measure the ethanol concentration (refer to criteria in Chapter 4, section 4.4.7.1).

7.2.3 Assessing Inventory-Constraint Controlled Variables via I_{VV} Index

It is important to assess whether it is sufficient to control only two variables (L_1 and T_2) in order to meet both inventory and constraint control objectives. To understand the extent of interaction among the variables, we need to employ the analysis based on the variable-variable interaction index (Chapter 4).

Now, let the inventory-constraint variables:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} L_1 \\ L_2 \\ T_1 \\ T_2 \\ Et_2 \end{bmatrix} \quad 7-1$$

Then, the values of closeness index of each variable are combined to form the variable-variable interaction index (I_{VV}) as follows:

$$I_{VV} = \begin{bmatrix} \mathbf{0.00} & 0.00 & 0.19 & 0.29 & 0.13 \\ 0.00 & \mathbf{0.00} & 0.19 & 0.29 & 0.13 \\ 0.11 & 0.11 & \mathbf{0.00} & 0.08 & 0.16 \\ 0.10 & 0.10 & 0.05 & \mathbf{0.00} & 0.08 \\ 0.17 & 0.17 & 0.38 & 0.49 & \mathbf{0.00} \end{bmatrix} \quad 7-2$$

Note that, the first row indicates the effect of L_1 in the directions of the other variables i.e. $\delta_{11}, \delta_{12}, \delta_{13}, \delta_{14}, \delta_{15}$. Notice that the closeness index of a variable with respect to itself is always zero i.e. $\delta_{11} = \delta_{22} = \delta_{33} = \delta_{44} = \delta_{55} = 0$. Also notice that the closeness index of L_1 and L_2 or vice versa is zero ($\delta_{12} = \delta_{21} = 0$). Thus, this means that at steady-state L_1 and L_2 completely tract each other i.e. referred to as *perfect* variables interaction.

Because of perfect variables interaction between L_1 and L_2 , the values of their closeness index with other variables are also the same. Thus, from steady-state point of view, it does not matter whether we choose L_1 or L_2 as a controlled variable because their impacts on other variables are expected to be almost the same.

Now, let compare the influences of T_1 and T_2 on the other variables by looking at the 3rd and 4th rows respectively. If we make a comparison based on the column values (i.e. column by column then, subsequently, row by row comparison), then obviously that the values in the 4th row are smaller (ignore the variable own closeness index i.e. 0 value) than that in the 3rd row.

What does this mean? This implies that T_2 has more influence on the other variables than T_1 has. Therefore, it is justified that T_2 is chosen as the constraint controlled variable because not only it is the most critical constraint variable (from the heuristic analysis point of view) but also it has the most influence on other variables (i.e. values of its closeness index are small).

Next question, is it sufficient to control only T_2 ? To answer this question let invoke the algorithm for analyzing the variable-variable interaction described previously in Chapter 4 (Section 4.4.7.2). Let the maximum threshold value of the closeness index be 0.09 i.e. $\delta_{max} = 0.09$.

After selecting T_2 as the controlled variable, let us check the maximum value in the 4th row (i.e. corresponding to T_2):

$$I_{4,max} = \max_{\delta_{ij}|j=1\dots5} (I_{VV}|_4) = \max(0.10, 0.10, 0.05, 0.0, 0.08) = 0.10$$

Since $I_{4,max} > \delta_{max}$, this means that we need another controlled variable. Upon inspection of the 4th row of I_{VV} (Eq. 7-2), we notice that the values of closeness index of T_2 with L_1 and L_2 are (largely) responsible for $I_{4,max} > \delta_{max}$. Thus, our target is to control either L_1 or L_2 . As mentioned previously that there is no difference either we choose L_1 or L_2 from the steady-state point of view. However, it is more advantageous to control L_1 than L_2 because the former will lead to faster dynamic response. In the next dynamic simulation study, we will evaluate the effectiveness of controlling either L_1 or L_2 . To complete the variable-variable interaction analysis above, let say we choose L_1 as the next controlled variable.

Now, we examine the maximum value of closeness index in the 1st and 4th rows.

$$\begin{aligned} I_{14,max} &= \max_{\delta_{1j}, \delta_{4j}|j=1\dots5} \left[\min_{\delta_{l1}|l=1,4} (I_{VV}|_{1,4}^1), \dots, \min_{\delta_{5l}|l=1,4} (I_{VV}|_{1,4}^5) \right] \\ &= \max(0.0, 0.0, 0.05, 0.0, 0.08) = 0.08 \end{aligned}$$

Obviously, with L_1 and T_2 chosen as the controlled variables, $I_{14,max} < 0.09$ hence, this indicates that it is sufficient to control only these two variables (out of five variables). Of course, the other uncontrolled variables will be indirectly controlled to within an acceptable range of variations by virtue of their closed interaction with these two controlled variables.

7.2.4 MIMO Controller Pairings and Tunings

Two control structures (with 4x4 dimension) are selected with controlled variables as shown in Table 7.1. Both have 2 primary controlled variables to achieve the overall performance measures (as in Chapter 6), 1 variable to achieve inventory control and 1 variable to achieve constraint control objectives. The key difference between the two control structures lies in the selection of controlled variable to achieve the inventory control objective i.e. while L_1 is used in CS1 and L_2 is used in CS2.

The manipulated variables for both control structures are (1) fresh feed flowrate F_o , (2) vapor flowrate from the vacuum flash vessel F_v , (3) cell recycle ratio R , and (4) outlet flow from the first bioreactor F_1 . Here, the selection of manipulated variables from 6 potential inputs is done via process knowledge. No attempt to employ more rigorous tools such as *Morari Resiliency Index* is made in this study.

The Bristol's *RGA* analysis is adopted in order to determine the manipulated-controlled variables pairings. The steady-state gains used to perform the *RGA* analysis are obtained from the transfer functions of the linearized plant model. Table 7.2 shows the *RGA* values for both control structures. Based on the *RGA* values, the controller pairings are as shown in Table 7-3.

Figure 7-2 and Figure 7-3 show the schematics of control structure # 1 (CS1) and control structure #2 (CS2) for the TSCE alcoholic fermentation system. The main difference between CS1 and CS2 lies in the choice of controlled variable for inventory control. While the CS1 adopts L_1 as controlled variable, CS2 adopts L_2 as controlled variable to achieve inventory control objectives. However, both use similar manipulated variable which is the fresh substrate flow F_o .

Table 7-1: Two control structures of complete partial control design

Control Structure	Primary Controlled Variables		Inventory Control	Constraint Control
CS1	S_2	rx_2	L_1	T_2
CS2	S_2	rx_2	L_2	T_2

Table 7-2: RGA values of CS#1 and CS#2

CS1					CS2				
	F_o	F_v	R	F_1		F_o	F_v	R	F_1
S_2	4.67	-0.43	2.59	-5.82	S_2	-0.88	0.30	2.3	-0.72
rx_2	-13.0	0.86	-1.68	14.8	rx_2	0.79	-0.37	-1.24	1.82
L_1	8.00	-0.05	0.16	-7.11	L_2	0.98	-0.01	0.02	0.05
T_2	1.34	0.62	-0.06	-0.90	T_2	0.11	1.08	-0.08	-0.11

Table 7-3: Controller pairings

Control Structure	Primary Controlled Variables		Inventory Control	Constraint Control
CS1	R- S_2	F_1 - rx_2	F_o - L_1	F_v - T_2
CS2	R- S_2	F_1 - rx_2	F_o - L_2	F_v - T_2

Table 7-4: Controller tuning values for CS#1 and CS#2

CS1	
R- S_2	$-(1.328s + 0.492) \times 10^{-4}/s$
F_1 - rx_2	$(13s + 11)/s$
F_o - L_1	120
F_v - T_2	-4
CS2	
R- S_2	$-(1.328s + 0.492) \times 10^{-4}/s$
F_1 - rx_2	$(9s + 5)/s$
F_o - L_2	20
F_v - T_2	-4

7.2.5 Selection of Controller Algorithm and Tuning

We choose PI controllers to control the primary controlled variables (S_2 and rx_2) whereas P-only controllers are adopted for the inventory and constraint control. The main reason for adopting PI controllers is to ensure no offset in the primary controlled variables.

Sequential loops closing is applied beginning with the two primary control loops, followed by the inventory and lastly by the constraint control loop. Initial tuning values are obtained from the IMC tuning formula with conservative tuning.

To obtain the initial tuning values, IMC tuning formula is adopted based on the simple first order plus deadtime (FOPDT) models identified at the nominal operating level. Then, the controller tuning values are refined to achieve an acceptable dynamic performance in term of disturbance rejection. Table 7-4 shows the controller tuning values for both control structures. The tuning values for the R - S_2 and F_v - T_2 control-loops are the same for both control structures. Different tuning values are used for the F_I - rx_2 and F_o - L_2 control-loops.

7.3 Dynamic Simulation of CS1 and CS2 Partial Control Strategies

7.3.1 Dynamic Responses of Primary, Constraint and Inventory Controlled Variables

The performances of the two control structures against step disturbance in S_o with magnitude of 30 kg/m^3 are tested. Figure 7-4 shows the dynamic responses of S_2 , rx_2 , T_1 , T_2 , L_1 and L_2 . The responses of S_2 and rx_2 are quite comparable in term of settling time under both control structures. But the responses of S_2 and rx_2 tend to be oscillatory under CS2 when subject to step decrease in S_o . Note that, the pattern of S_I profile follows closely that of S_2 i.e. as predicted from the previous PCA analysis (Chapter 6) where these two variables are found to be closely correlated.

As for the bioreactor temperatures, it can be observed that the fluctuation of T_2 (peak value) under CS1 is smaller than under CS2. This is very desirable as the peak value of temperature should not exceed 33°C , otherwise the yeast cells will be damaged, which in turn can reduce the yield and productivity of ethanol.

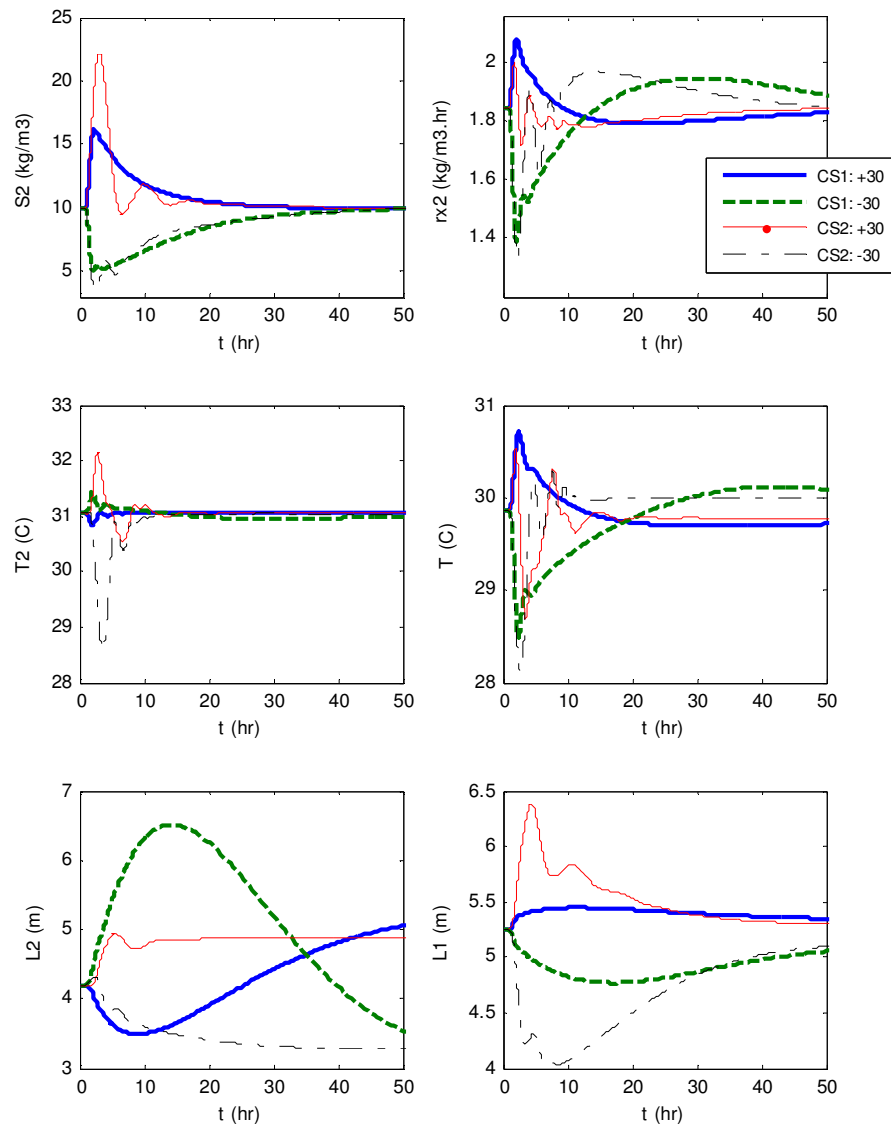


Figure 7-4: Responses of the primary controlled variables when subject to step changes in S_0 of $\pm 30 \text{ kg/m}^3$

Interestingly, the response of T_1 is quite comparable under both control structures except it tends to show more oscillatory behaviour under CS2. Note that, T_2 is the controlled constraint variable under both CS1 and CS2 and T_1 is uncontrolled variable. Notice that, both constraint variables are having peak values which are below 33°C with T_2 having the smallest peak under the CS1 strategy.

Unlike S_2 and rx_2 which exhibit quite similar profiles under both control structures, the dynamic responses of L_1 and L_2 under both control structures show different profiles. For CS1 where L_1 is the controlled variable for the inventory control objective, its fluctuation is smaller than that under CS2 where the L_2 is the controlled inventory variable. On the other hand, the reverse pattern is observed for L_2 under CS2 where it is directly controlled. Despite the difference in peak (fluctuation) values, the responses of L_1 and L_2 show quite similar settling time and steady-state offset.

Surprisingly, under CS1 the direction or trend of the dynamic responses of L_1 and L_2 is opposite to each other. This is in contradiction with the result of PCA-based analysis which shows that they are positively correlated; so, they should exhibit similar dynamic trend or similar direction. Now, obviously the implementation of the control structure CS1 has changed the nature of variables interaction – open-loop variables interaction is not the same as that of closed-loop especially under CS1. On the other hand, the profiles of these variables exhibit quite a similar trend under CS2. Thus, it seems that the implementation of CS1 has reversed or even broken this correlation. Furthermore, this suggests that the variables interaction under the open-loop can be different from that under the closed-loop. And of course, when the system is in closed-loop, the variables interaction can depend on the type of control structure implemented as well e.g. CS1 and CS2 lead to different closed-loop variables interaction characteristics.

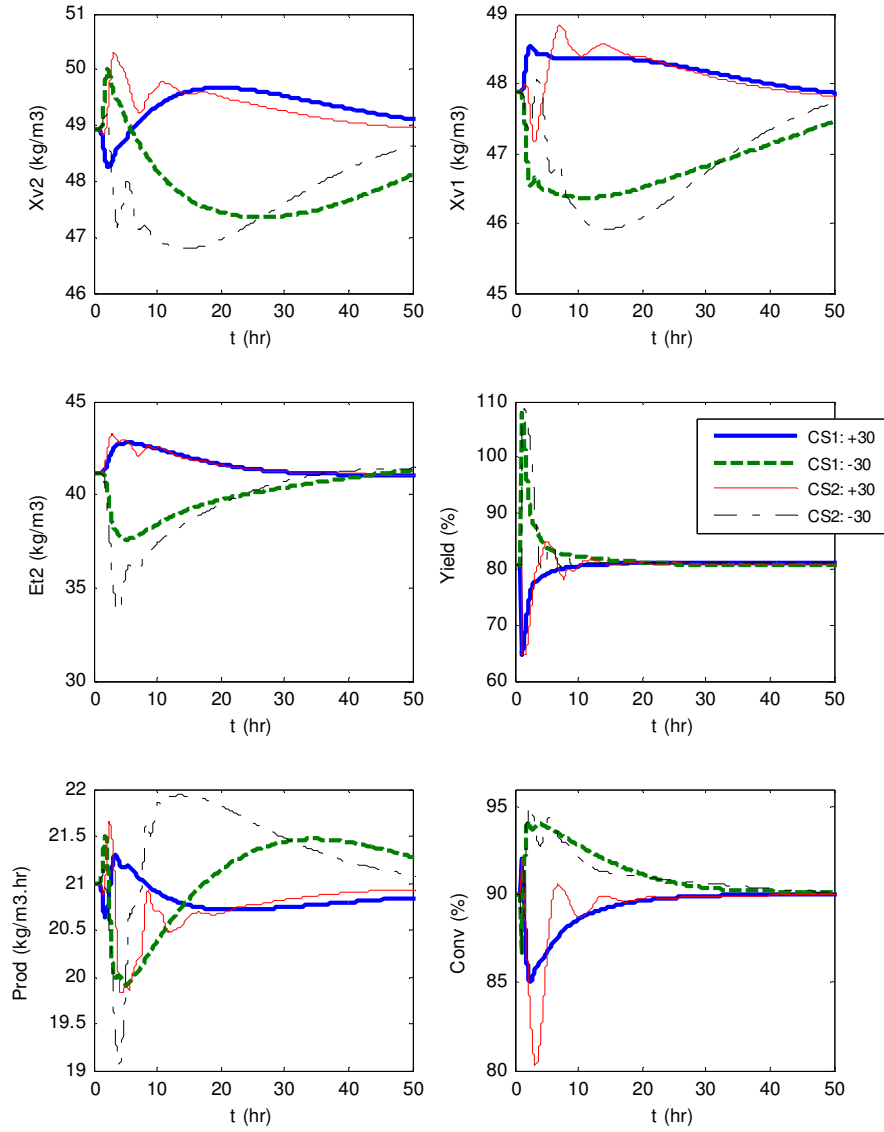


Figure 7-5: Responses of uncontrolled output variables and performance measures when subject to step changes in S_o of $\pm 30 \text{ kg/m}^3$

7.3.2 Dynamic Responses of Uncontrolled Variables

Figure 7-5 shows the profiles of X_{v1} , X_{v2} and Et_2 which are the uncontrolled variables. The responses of these uncontrolled variables are quite sluggish and seem to be comparable under both control structures i.e. no advantage is shown by either control structure. It is rather surprising that the response of Et_2 does not seem to strongly follow the profiles of L_I under CS1 i.e. CS1 changes the nature of open-loop variables interaction.

Therefore, in other words this means that the correlation of Et_2 with L_I (refer to Figure 7-4) has somehow been broken or at least weakened by the implementation of CS1. Based on the previous PCA-based analysis, these two variables are positively correlated. And yet by comparing the profiles of Et_2 with L_I (see Figures 7-4 and 7-5 respectively), we can notice that they show the opposite trends during the transient stage. In turn, this shows that the different nature of variables interaction could arise depending on whether the system is open-loop (former case) or closed-loop.

In conclusion, there is no advantage of adopting either control structure in terms of X_{v1} , X_{v2} and Et_2 dynamic responses. This is because under both control structures, the dynamic responses and offsets are quite comparable.

7.3.3 Dynamic Responses of Performance Measures

The responses of performance measures can be observed in Figure 7-5, when subject to the disturbance. From the *Yield* response perspective the performance of CS1 and CS2 are almost comparable. Similarly from the *Conv* dynamic response perspective, both control structures are comparable but CS2 shows larger undershoot value when subject to step increase in S_o . This implies under CS2 there will be a severe drop in conversion followed by sluggish recovery to about the nominal operating value.

It is interesting to note that, CS1 shows markedly better performance in term of *Prod* response – i.e. faster recovery of *Prod* under CS1 than under CS2. In contrast, large undershoot value of *Prod* occurs under the CS2 when subject to step decrease in S_o implying heavy loss in productivity before it is slowly restored to about its nominal operating value. It is important note that, the offsets or steady-state variations in

performance measures are smaller than the maximum allowable variation of 1.0% under both control structures i.e. offsets are less than 0.4% - thus, almost comparable with the previous basic partial control strategy (Chapter 6).

7.3.4 Summary of Dynamic Simulation Results

From the dynamic simulation results, we can draw an overall conclusion that the CS1 exhibits better performance than CS2 in terms of:

- 1) Faster responses of the performance measures especially the response of *Prod* (productivity), smaller undershoots of *Conv* (conversion) and *Prod*.
- 2) Faster response of the constraint control (T_2) and smaller overshoot value of T_2 i.e. maximum peak is less than 33°C.

However, CS2 shows slightly better performance from the inventory control perspective because it leads to smaller maximum peak value of liquid level. This is advantageous in the sense that it allows us to use smaller bioreactor or to operate closer to the maximum capacity of the bioreactor. One main reason why liquid levels fluctuate less under the CS2 than under the CS1 is that, in the former the strong positive correlation (open-loop variables interaction) between L_1 and L_2 are maintained. On the contrary, their interaction seems to be reversed under the latter. We will further discuss the impact of changing the variables interaction in the next Chapter 8.

In the next section, we will discuss how to enhance the dynamic performance of CS1. Thus, the CS2 will not be discussed anymore from this point onward.

In the subsequent section, our main objective is to improve the performance of CS1 in terms of the following:

- a) The achievement of faster dynamic recovery of the performance measures.
- b) The reduction of the *highest peak* overshoot of the liquid level i.e. L_2 .

7.4 Performance Enhancement of Partial Control

There are various methods which could be employed in order to enhance the PID performance and among the most common approaches are (1) feedforward control, (2) cascade control, and (3) ratio control. Other approaches include the (1) decoupler to reduce loops interactions, (2) robust-loop shaping to improve the trade-off between performance and robustness, (3) delay compensation to overcome limitation arising from long deadtime, and many more.

In this study, we will focus on the possibility of implementing the most commonly adopted approaches in industry namely, the feedforward, cascade and ratio controls. Additionally, because each technique is suitable for certain types of disturbance, it is important to decide which technique is the most suitable for a particular process of interest.

7.4.1 Selection of PID Enhancement Techniques

To determine which technique is the most suitable for our application, the following simple steps are employed:

Step 1: Identify types of disturbances

In order to select the most appropriate enhancement technique, we need to identify the types of disturbances and how they affect the key process variables (primary, inventory or constraint). In this case study, the main disturbance is the fresh substrate concentration S_o and it has a direct effect on the primary variable S_2 . In addition, it also has strong effect on rx_2 but its influence on this variable is presumably slower than on S_2 . Because S_o has influence on the fermentation kinetics (i.e. not only on the growth rate but also on the substrate consumption and product formation rates), then its fluctuation tends to influence the constraint variable T_2 , which can cause the violation of the threshold value for this variable. Thus, it is very desirable to reduce the effect of S_o disturbance on the system.

Step 2: Identify control-loop to be enhanced

To identify which control-loop to be enhanced, we need to know which of the controlled variables strongly influence the key performance measures i.e. the primary controlled

variables. There are two control-loops that strongly influence the performance measures, which are F_I-rx_2 and $R-S_2$. Note that in term of ranking, S_2 has stronger influence on the key performance measures than rx_2 . Thus, our target is to enhance the dynamic performance of $R-S_2$ control-loop.

Step 3: Identify suitable enhancement technique

Ratio Control

Based on this disturbance type, ratio control is rejected because it is only suitable for flow disturbance which can scale directly with the manipulated variable (R). In this case, the concentration (S_o) does not scale directly with the manipulated variable. Hence, the ratio control will not work for our application.

Cascade Control

There is a possibility to use cascade control by cascading S_2 (controlled variable for master controller) with S_I (controlled variable for slave controller). The reason for this is that the disturbance which enters the first bioreactor will affect S_I first before affecting S_2 in the second bioreactor. Therefore, by controlling S_I with slave controller, we can reduce the impact of disturbance on S_2 . However for this scheme to work, the inner loop involving S_I must be at least 3 times as fast as that of the outer loop involving S_2 . To assess the speed of responses of S_I and S_2 , an open-loop step test is conducted by increasing R by 0.05.

Figure 7-6 shows the open-loop responses of S_I and S_2 to step change in R . From the figure, it can be seen that the open-loop dynamic responses of S_I and S_2 are comparable. Consequently, this suggests that it is rather unlikely for the inner loop of the cascade control to be at least 3 times as fast as that of the outer loop. Therefore, cascade control technique is not suitable for our case.

Feedforward Control

Having rejected ratio and cascade control strategies, we are left with feedforward control. For feedforward control to work, we need an approximate (linear) model (i.e. transfer function) relating the S_o to S_2 . Additionally, provided that we have a measurement of the disturbance, it should be relatively straightforward to apply the feedforward control strategy in this case. Accordingly in our case we will adopt the feedforward control strategy to enhance the dynamic performance of CS1.

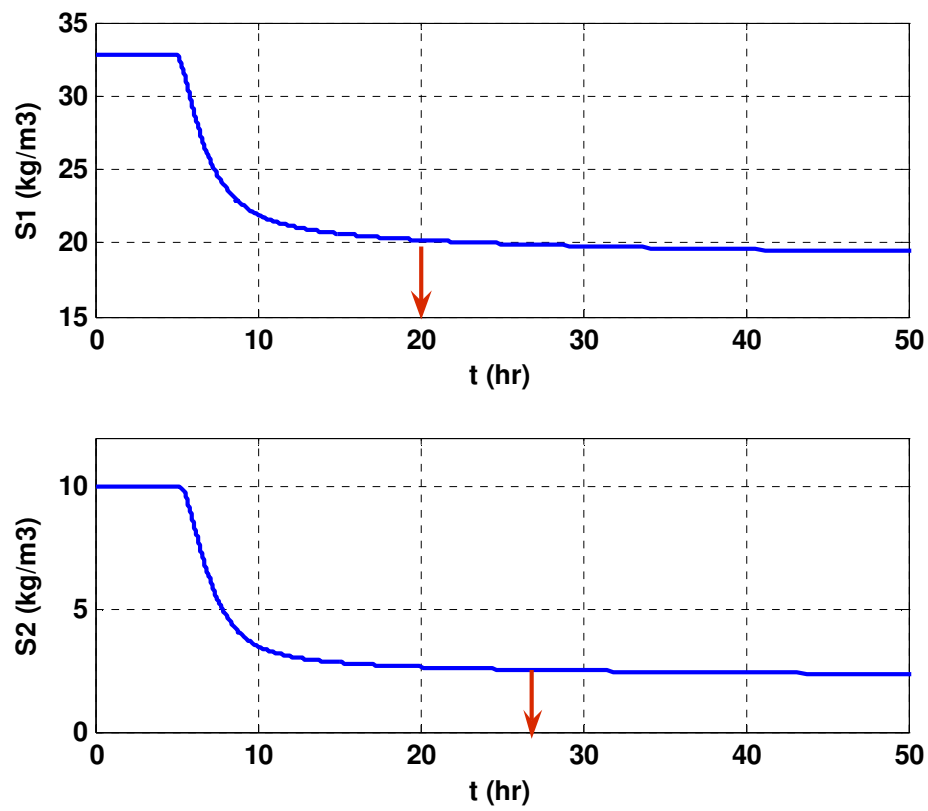


Figure 7-6: Open-loop responses of S_1 and S_2 to step change in R by 0.05 (arrow indicates settling time)

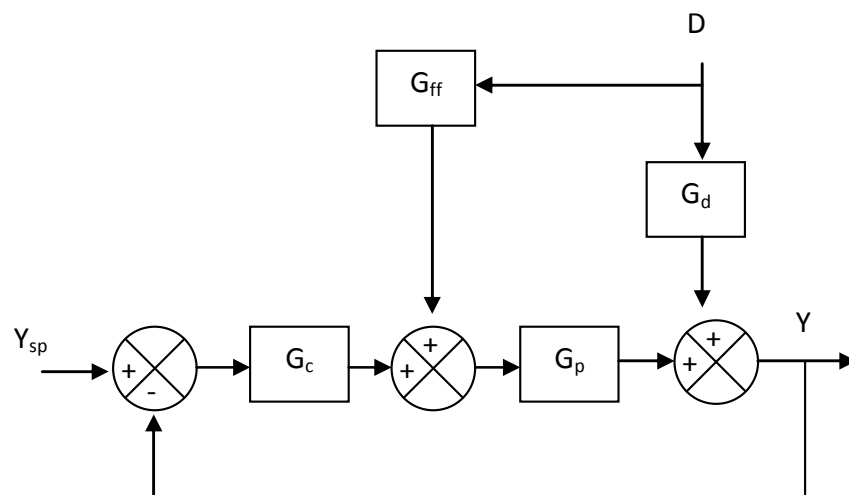


Figure 7-7: Block diagram of combined feedback-feedforward control (Riggs and Karim 2006)

7.4.2 Design of Feedforward Controller

To design the feedforward (FF) controller, transfer function models are developed based on step test procedure. This leads to two models, one for disturbance (S_o), and another for the manipulated variable (R) impacts on S_2 i.e. $G_d(s)$ and $G_p(s)$ respectively. At the nominal operating conditions, the step test yields the following two models:

$$G_d(s) = \frac{S_2(s)}{S_o(s)} = \frac{0.8}{(2.0s+1)} \quad 7-3$$

$$G_p(s) = \frac{S_2(s)}{R(s)} = \frac{-14.5}{(2.7s+1)} \quad 7-4$$

The dynamic responses to develop the transfer functions above are shown in Figure 7-8. Bear in mind that, the models developed here are only crude approximation. Higher order models can be developed but can lead to more complex FF control algorithm.

Notice that from Eq. 7-1 and Eq. 7-2, the dynamic impacts of S_o and R are significantly different (i.e. R has slower impact on S_2). This suggests that a dynamic feedforward controller is required instead of a static feedforward controller.

Feedforward control can be synthesized based on the block diagram shown in Figure 7-7. The objective of feedforward controller G_{ff} is to compensate for the impact of disturbance D on Y . This can mathematically be written as follows:

$$G_{ff}(s)G_p(s)D(s) + G_d(s)D = 0 \quad 7-5$$

Thus, the feedforward controller is:

$$G_{ff}(s) = (-G_d(s))/(G_p(s)) \quad 7-6$$

Using this formula, we can derive the required feedforward controller for our case study based on the transfer functions obtained previously, which gives:

$$G_{ff}(s) = ((2.03s + 0.7))/((283s + 141.5)) \quad 7-7$$

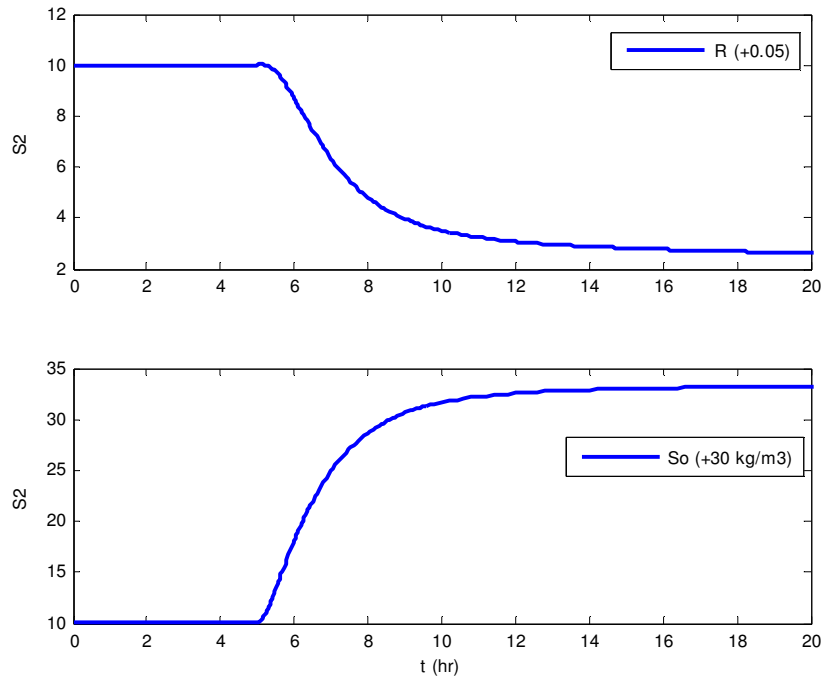


Figure 7-8: Step responses (open-loop) of substrate concentration in bioreactor 2 to step changes in R (by 0.05) and in S_0 (by 30 kg/m³)

Figure 7-9 shows the schematic of CS1 enhanced with FF control strategy. Note that, a slight change to CS1 is made where a PI controller is used to control the liquid level L_l instead of P-only controller. The revised tuning values for the feedback controllers augmented with the FF control are shown in Table 7.5.

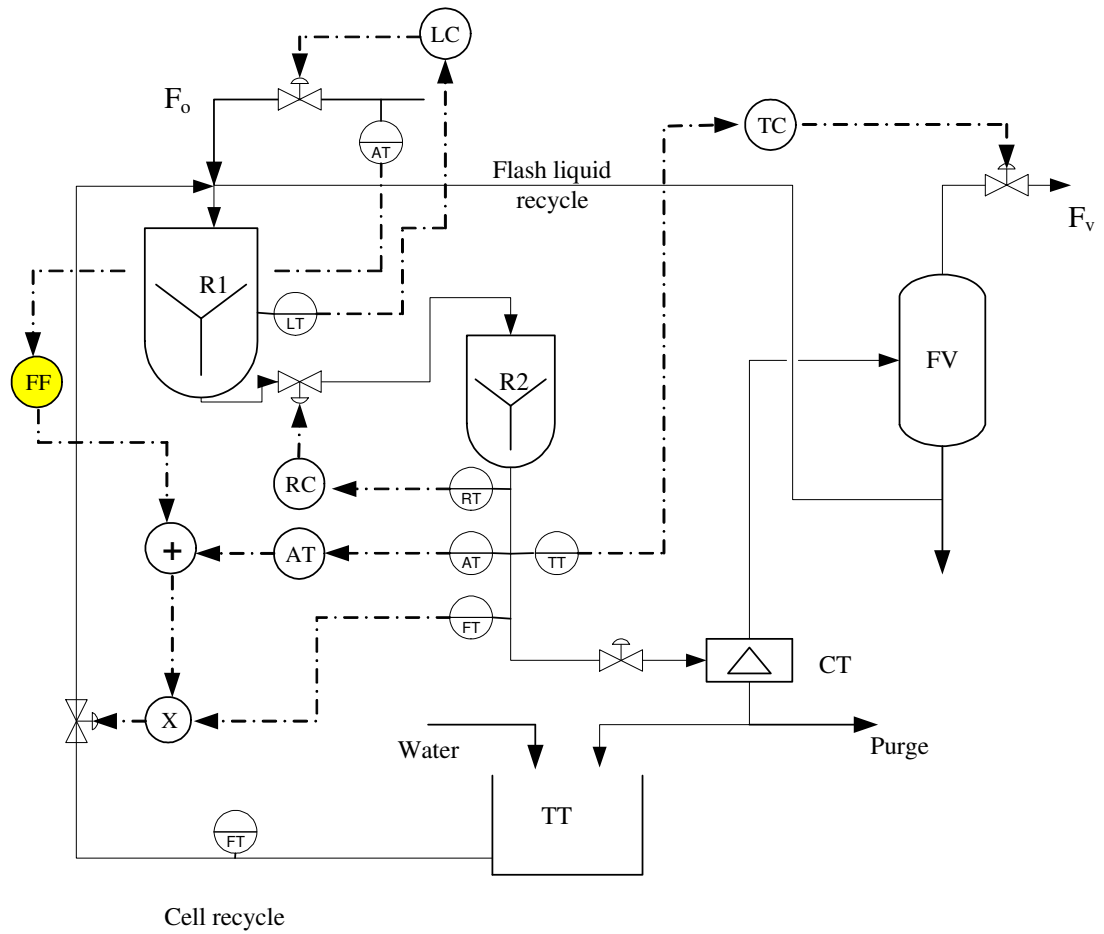


Figure 7-9: Schematic diagram of CS1 augmented with FF control strategy

Table 7-5: Controller tuning values for CS1 with feedforward (FF) control

Control-Loop	Controller Tuning
R-S ₂	$-(1.33s + 0.49) \times 10^{-4}/s$
F ₁ -rx ₂	$(26s + 8)/s$
F ₀ -L ₁	$(400s + 360)/s$
F _v -T ₂	-4

7.5 Dynamic Simulation with Feedforward Control Enhancement

7.5.1 Dynamic Responses of Primary Controlled Variables

Figure 7-10 shows the comparison of dynamic responses of the controlled primary variables for CS1 with and without feedforward (FF) control enhancement. With the feedforward control, S_2 settles down in less than 10 hours while it takes about 25 hours for the case without feedforward control. Thus, it shows that a significant dynamic improvement can be achieved with the feedforward enhancement for the S_2 response. Similarly, the implementation of FF controller also leads to faster dynamic response of the rx_2 .

Another interesting result arising from the feedforward enhancement is that the peak values (or overshoots or undershoots) in S_2 and rx_2 are slightly larger than without feedforward enhancement. Thus, it is expected that overshoots or undershoots of the performance measures will be slightly larger than without FF controller. Note that, the response of S_1 (not shown) follows closely that of S_2 as in the previous case of basic partial control (Chapter 6).

7.5.2 Dynamic Responses of Inventory Variables

The dynamic responses of liquid levels (inventory variables) in the bioreactors with and without feedforward control enhancement are shown in Figure 7-10. The settling time of the L_1 (controlled inventory variable) is much shorter with the feedforward enhancement than without feedforward. However, the dynamic response of the uncontrolled L_2 is only slightly faster with the feedforward control strategy.

With feedforward controller the overshoots in L_1 is only about 2%. Although FF controller can significantly improve the response of L_1 , its implementation seems to have marginal improvement on L_2 in term of reducing its overshoot value. Thus, we can draw a conclusion that FF controller only provides significant improvement for L_1 in terms of (1) faster dynamic response, (2) smaller overshoot or variation than the strategy without FF controller.

7.5.3 Dynamic Responses of Constraint Variables

Notice that from Figure 7-10, just like in the case of primary and inventory variables (i.e. L_I), the dynamic responses of the bioreactor temperatures are faster with the FF controller than without the FF enhancement. Surprisingly, the peak value of T_2 with the FF controller is larger than without FF controller. But the peak value remains well below the threshold value of bioreactor temperature i.e. $< 33^\circ\text{C}$.

7.5.4 Dynamic Responses of Biomass Concentrations

Note that, we decided not to control the viable cell and ethanol concentrations in both bioreactors. It is interesting to know how they respond to the disturbance change. Figure 7-11 displays how viable cell concentration (X_{v2}) responds to the disturbance under the CS1 with and without FF controller. Obviously, with FF controller the dynamic response of X_{v2} is very fast and with low maximum variations as compared to CS1 without FF enhancement.

Just like X_{v2} , with FF controller the dynamic response of Et_2 is also very fast as compared to that without FF controller (Figure 7-10). Also note that, the peak value of Et_2 with FF controller is much smaller than that without FF controller. Thus from this perspective, with the FF control enhancement we can greatly improve another constraint control objective (i.e. other than T_2), which is to minimize the peak variation in Et_2 .

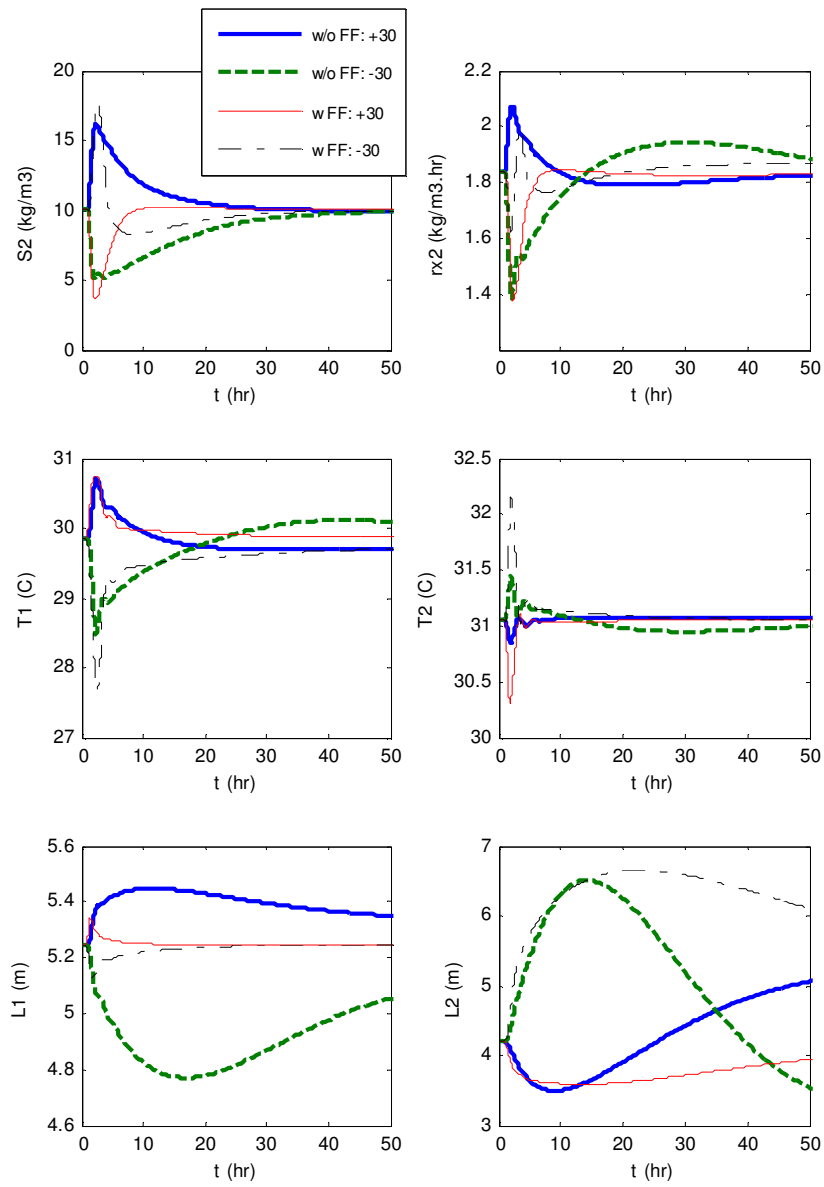


Figure 7-10: Responses of primary, constraint and inventory variables under CS#1 with and without feedforward control enhancement.

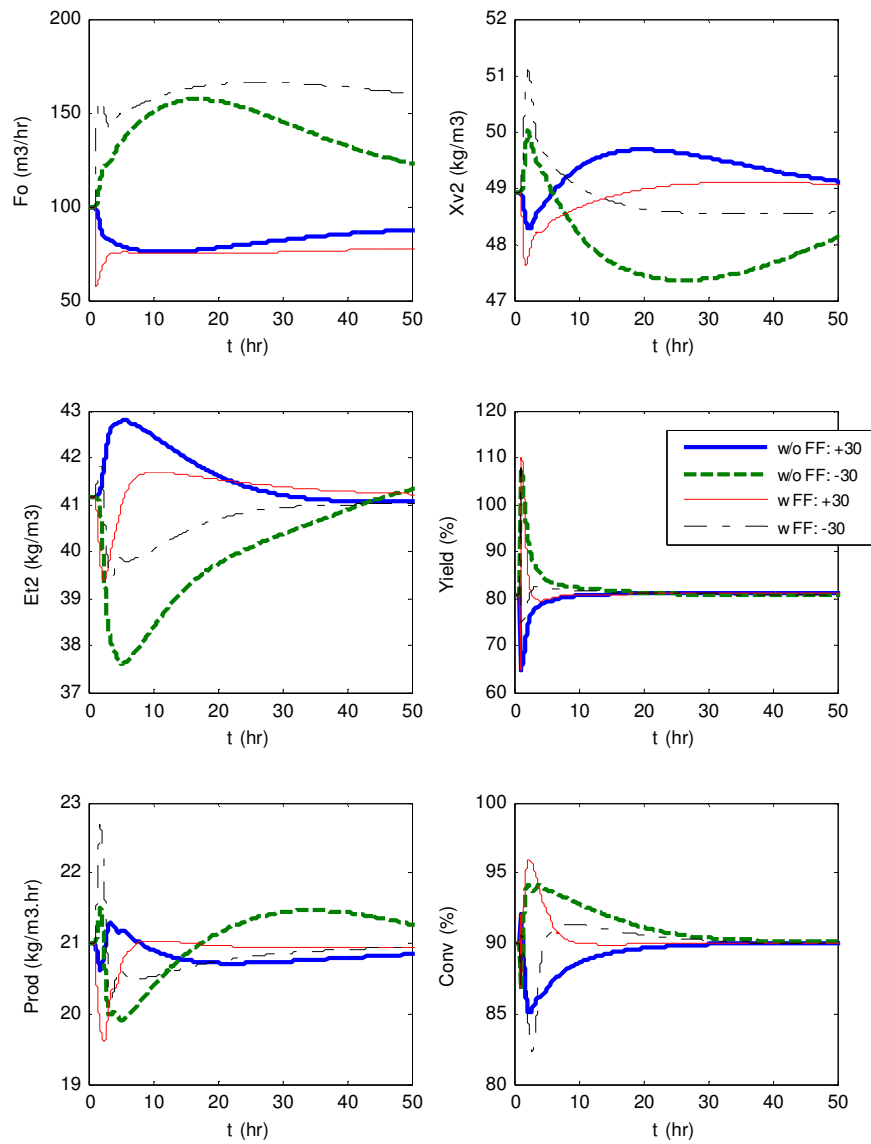


Figure 7-11: Responses of liquid levels under CS#1 with and without feedforward control enhancement.

7.5.5 Dynamic Responses of Performance Measures

Next, we look into the impact of FF control enhancement on the performance measures themselves i.e. *Yield*, *Conv* and *Prod*. Figure 7-11 shows how the three key performance measures respond to the step disturbance in S_o .

The dynamic response of *Yield* with the FF control enhancement is about twice as fast as that without FF controller (shorter recovery time with FF controller). On the other hand, both *Prod* and *Conv* show a significant improvement in their dynamic performance (i.e. faster recovery and lower peak variations) with FF controller. Furthermore, with FF controller the *Prod* and *Conv* can achieve recovery in about 10 hours after the step disturbance occurrence. Meanwhile for the case without FF controller, the recovery times for the *Prod* and *Conv* are about 70 and 30 hours, respectively.

7.5.6 Variations in Performance Measures

Table 7-6 shows the steady-state variations or offsets of *Yield*, *Conv* and *Prod* when subject to the step change in S_o by $\pm 30 \text{ kg/m}^3$. Notice that, the offsets of the performance measures for both CS1 and CS2 are comparable. But the basic partial control structure (Chapter 6) seems to show markedly better performance than either CS1 or CS2 in terms of the offsets – i.e. the former has smaller offsets. Nonetheless, all control strategies result in steady-state variations that are less than the maximum allowable limit of 1.0%.

Table 7-6: Steady-state offsets of key performance measures

Control Structure	$\Delta\text{Yield (\%)}$	$\Delta\text{Conv (\%)}$	$\Delta\text{Prod (\%)}$
CS1	0.01	0.01	0.35
CS2	< 0.01	0.01	0.25
CS1 w FF	0.03	<0.01	<0.01
Basic Design	<0.001	<0.01	<0.01

7.5.7 Summary of PID Enhancement Results

Overall when the CS1 is augmented with FF controller, we can gain the following improvements:

- i. Recovery times of *Prod* and *Conv* can be reduced by about 3 and 7 times respectively – i.e. faster disturbance rejection effect on performance measures.
- ii. Faster dynamic responses of liquid levels.
- iii. Faster dynamic responses of bioreactor temperatures and ethanol concentrations, hence better constraint control performance.
- iv. Faster dynamic responses of primary controlled variables and other uncontrolled variables.

7.6 Limitations of PID Enhancement Technique

It is important to note that, the variables interaction depend on the control structure design. Recall previously that while CS2 preserves the open-loop variable interaction, CS1 somehow alters this interaction. Thus, while under CS2 control strategy L_1 and L_2 remain positively correlated as in the open-loop case, these variables are found to be negatively correlated under CS1.

An important question is whether this change in variables interaction has any implication on the overall control performance. If it does, in what way this change affects the performance. Notice that from the dynamic simulation of PID enhancement, some of the unexpected things happen, for example, the dynamic response of L_2 shows no improvement at all with the implementation of FF controller. Furthermore, the peak fluctuations (overshoots or undershoots) remain as high as that without FF control enhancement. As a result of this, we could not operate the second bioreactor close to its maximum volume. Note that, it is always desirable to operate the bioreactor close to its maximum volume because it can lead to maximum economic benefit. Unfortunately, high fluctuations in liquid level definitely prevent the operation close to the maximum bioreactor volume.

In view of the above mentioned limitations, we will further investigate the impact of variables interaction in the next Chapter 8. The primary motivation for this further investigation is to explore whether the dynamic performance can be further improved if the variables interaction can be preserved i.e. open-loop variables interaction similar to closed-loop variables interaction.

7.7 Non-uniqueness of DV Sets by Classical Definition

From the classical dominant variables definition point of view, the subset $\{L_1, T_2\}$ or $\{L_2, T_2\}$ can be considered as the dominant variable (DV) sets because of acceptable variations of other variables can be ensured by controlling them. But of course in view of the strong correlations of variables in $\{Et_2, L_1, L_2, T_1, T_2, F_0\}$, we could also propose other subsets of variables to be controlled such as $\{L_1, Et_2\}$, $\{T_2, Et_2\}$, $\{L_2, Et_2\}$ and many more. As far as the classical definition is concerned, all of these subsets are

qualified as DV sets – i.e. by controlling them we can more or less ensure acceptable variations in the other uncontrolled variables. It seems obvious that, there is no unique subset of DV as far as the classical definition is concerned. Consequently, this non-uniqueness of DV sets from the classical framework of partial control leads to 2 major implications:

- 1) Because there are many candidates for DV sets, it is not hard to understand why engineers can successfully apply partial control even without systematic tool i.e. just following engineering intuition or process knowledge. However, engineers will be expected to encounter great difficulty when attempting to obtain the dominant variables for the implicit operating objectives e.g. optimum profit, minimum cost, optimal trade-off between two or more contradicting objectives such as in this case study. In other words, it is far from obvious how to identify the *implicit* variables which have the dominant effects on the performance measures.
- 2) Engineers have often ignored the benefits of interaction among the variables. Understanding this interaction can lead to less number of controlled variables, which in turn leads to simpler control structure. Take for example in this case study, if we have no clue what so ever regarding the interactions among the variables, then we tend to be more conservative by attempting to control more variables e.g. to control three or four variables instead of only two variables (i.e. 1 constraint and 1 inventory controlled variables). Therefore, the implementation of partial control based on process knowledge and experience could yield *workable* control strategy, but in the absence of good knowledge regarding the variables interaction we expect the result tends to be conservative – we tend to control more variables than are necessary.

Bear in mind that to clear this confusion, in this thesis the dominant variables are defined only for the overall performance measures or operating objectives which are the implicit functions of process variables/ parameters i.e. new definition of dominant variable. As such, the subset $\{L_1, T_2\}$ for example, is not considered as the DV set because they relate to other process variables and not to the implicit performance measures. It is important to note that, the subset $\{L_1, T_2\}$ is selected as controlled

variables mainly as a result of the PCA-based analysis aided by some process understandings. Such selection of only fewer controlled variables than the output variables of interest to achieve the inventory and constraint control objectives is possible because of the *strong interaction* among these variables. Without the strong interaction among the variables, obviously we need to control more variables. Therefore, in order to assess the sufficient number of controlled variables, we can employ the variable-variable interaction analysis via the I_{VV} index. In this case we use a systematic tool to predict the extent of variables interaction and its impact on the number of controlled variables required.

7.8 Variables Interaction: Working Principle of Partial Control

Imagine that there is no interaction among the variables $\{Et_2, L_1, L_2, T_1, T_2, F_o\}$ in the sense that, whatever we do to one variable has no effect on other variables. For example, if T_2 is selected as a controlled variable, then other uncontrolled variables remain completely free to drift if there is no interaction between T_2 and these other variables. As a consequence, we need to control not only $\{L_1, T_2\}$ but also $\{Et_2, L_2, T_1\}$, as well which leads to five controlled variables instead of only two. As we have only four manipulated variables remaining, this means that we will face a great difficulty in trying to remove one of the controlled variables – and probably the result will not be too good either.

It has always been perceived that the adoption of partial control is necessary because of the less number of manipulated variables than the output variables. But it is very important to realize that the partial control itself is made possible because of the variables interaction. If the variables interaction does not exist, then, we are forced to control every output variables which are deemed important to the overall plant objectives including the inventory and constraint control objectives.

In this manner, the interaction among variables can be considered as the *working principle* in partial control strategy - partial control is governed by the variables interaction. An important implication of this principle is on the *optimal size* (i.e. total number of controlled variables or control-loops) of complete partial control structure. Hence, for the case where variables have strong interactions, the optimal size can be smaller than that for a case where the variables have weak interactions. Further

discussion on the implication of the size of partial control structure on the control system performance will be discussed in the next Chapter 8.

7.9 Understanding Variable Interaction by PCA-based Method

The idea of exploiting the interaction among variables to achieve control objectives is not new. In his “Critique of Chemical Process Control Theory” Foss (1973) mentioned that it is not necessary to make the process non-interacting simply because it is difficult to design multivariable control system by the single-loop methods. He further emphasized that the exploitation of interaction inherent in multivariable processes “*takes judgment, brains, and maturity and a good theory*”.

If the variable interaction can be so important, then it becomes necessary for engineers to understand such interaction and exploit its benefit. Other than for the input-output (I-O) variables interaction which is commonly addressed in controller pairings using the well known Bristol’s RGA analysis for example, we are short of systematic techniques to analyze the output-output (O-O) variables interaction. As has been argued in the previous Section 7.4.2, the understanding of O-O variables interaction is the key element in the proper design of partial control strategy.

Interestingly, the PCA-based method (Chapters 3 and 4) can systematically be used to understand the variables interaction, which is the key principle enabling the application of partial control structure. Understanding of this interaction can lead to proper (1) selection of controlled variables, and (2) determination of sufficient number of controlled variables that are just *sufficient* to achieve the control objectives (overall, inventory and constraint control objectives). In other words, we can avoid an overly complex design with too many controlled variables with the help of PCA-based method – thus, making it possible to design an optimal size partial control strategy.

7.10 Summary

We have shown in this chapter the application of the PCA-based method (i.e. data-oriented approach) to design complete partial control strategy incorporating the inventory and constraint control objectives (application of methodology described in Chapter 4). In the case study, both control structures without PID enhancement technique perform quite well but the control structure #1 (CS1) shows markedly better overall performance than that of CS2. The CS1 and CS2 are different only in term of the choice of inventory controlled variables; the former uses L_1 and the latter uses L_2 as a controlled variable to achieve the inventory control objective.

Furthermore, we also propose a simple procedure that could be used to select the appropriate PID enhancement techniques. This procedure is applied in order to enhance the performance of CS1, which leads to the selection of feedforward control strategy. It is found that the feedforward control enhancement provides significant improvements over CS1 without PID enhancement as follows:

- 1) Faster recovery in performance measures.
- 2) Faster responses in controlled and uncontrolled variables.
- 3) Lower peak values in bioreactor temperatures and ethanol concentrations.

An important conclusion which can be drawn from the simulation study is that the variables interaction is dependent upon the choice of control strategy or structure. In the case study, while CS2 preserves the open-loop variables interaction, the CS1 alters this interaction. In this chapter we have not yet established to what extent such an alteration in variables interaction affects the overall control performance. However, we expect this alteration has something to do with the lack of improvement in the inventory control performance under CS1 when it is augmented with the feedforward control strategy.

The idea of exploiting variables interaction to achieve control is not new as it was mentioned nearly 4 decades ago by Foss (1973) in his “Critique of Chemical Process Control Theory”. Surprisingly, the systematic tool which can be used to understand especially the output-output (O-O) variables interaction and exploit its benefits for control purposes has not yet been developed. Thus in view of this shortcoming, the PCA-based method described in this thesis is perhaps the first systematic technique, which can be employed to understand this interaction and to provide guideline on how to

exploit its benefits. One of the main benefits of interaction is that it allows us to control only small subset of variables to achieve a variety of control objectives. But of course, this leads to an important question which is how many controlled variables are sufficient to meet the specified control objectives. To answer this question we can employ the variable-variable interaction index I_{VV} to analyze the extent of variables interaction, which in turn allows us to unambiguously assess the sufficient number of controlled variables required.

Finally, we recognize that the variables interaction is the *governing* principle that enables the partial control idea to be applicable in real practice. Without this important property, partial control cannot be realized in many real cases – thus, understanding of the variables interaction is fundamental in the design of partial control strategy in particular and plantwide control in general.

8 OPTIMAL SIZE OF PARTIAL CONTROL STRUCTURE

8.1 Introduction

In Chapter 7, we have compared different types of partial control strategies with size of 4×4 . Note that, the size of the partial control design is given by the number of controlled variables, e.g. 4×4 implies 4 controlled variables are adopted. The results from the previous chapter showed that further closed-loop performance improvement can be achieved by incorporating the feedforward control into the partial control strategy. Also, the results showed that the partial control strategy with the feedforward enhancement (referred to as CS1 in Chapter 7) can in fact, achieve all three types of operating objectives: the overall, constraint and inventory control objectives.

Despite this wonderful result, we ask ourselves is there a way we can further improve the performance of CS1 control strategy? Specifically we are interested to reduce the peak fluctuations (changes) of the inventory variables such that in practice, this reduction allows us to operate closer to the maximum bioreactor volume. We are motivated to achieve this *extra* goal because by operating the bioreactor closer to its maximum volume, we can in practice achieve better economic performance. Of course, there could be several answers to the question mentioned above, for example, the applications of advanced controller algorithms (e.g. MPC), can be adopted in this case. But our quest to improving the CS1 in this study leads us to a rather different and unconventional direction – one that has never been reported in open literature before.

8.1.1 Conditions for Effective Partial Control Design

Our approach to improving the performance of CS1 strategy as described in this chapter arises from our understanding of the basic principle governing the way partial control works, and the reason for its implementation on a process system of interest. As a result

of this understanding, we propose two important conditions for an effective partial control design:

- 1) The control-loop which imposes limitation on the speed of (overall) dynamic responses must be eliminated – here, the limiting control-loop is referred to as the *bottleneck control-loop (BCL)*.
- 2) The open-loop variables interaction must be preserved (or its change be minimized) by the control system being implemented – ideally the open-loop and closed-loop should have similar nature of variables interaction.

8.1.2 Concept of Bottleneck Control-Loop (BCL)

In relation to the first condition, we propose a concept of *bottleneck control-loop (BCL)*. *Bottleneck control-loop* is defined as the loop which limits the dynamic response of the entire control system. This is quite similar to the idea of rate limiting step in serial chemical reactions. However, the key difference lies in the fact that BCL is not easily identified because of the intricate nature of interaction among the control-loops in the system. It is important to note that, the existence of BCL is caused by the interactions among the loops via the output-output variables (O-O variables) interaction. As a consequence, the more control-loops are there (larger size of control strategy) in the system, the more likely that the BCL presents in the system.

It is important to distinguish between the control-loops interaction and the variables interaction. In the former, the interaction arises from the coupling between the control-loops in a typically closed-loop system only – not applied to an open-loop system. On the other hand, the O-O variables interaction (especially among the output variables) exists for a closed-loop as well as for the open-loop systems. Recall from Chapter 7, this type of interaction depends on the choice of control structure; different control structures have different influence on variables interaction, which either preserve or alter the open-loop variables interaction.

In addition, unlike the control-loops interaction the implication of variables interaction on the design of control system is an area which is least studied. In so far, there has been no method available to deal systematically with the variables interaction. In the next sections, we will discuss and highlight the significance of BCL and propose a

method for its identification. But first let us introduce another concept namely the *synergistic external-inherent* control system.

8.1.3 Concept of Synergistic External-Inherent Control System

With regard to the second condition, another aspect which can lead to the sub-optimal performance of a partial control strategy that has been observed in this current study is the mismatch of the variables interaction between the open-loop and closed-loop situations. As a result of this observation, we propose that the significance of the variables interaction is strongly linked to the existence of *inherent* control system possessed by any (open-loop) process of interest. In general, most of real (multivariable) processes which are self-regulating can be considered as having the *inherent* control ability; otherwise, the system can be completely unstable or open-loop unstable. This inherent controller is one of the important characteristics of real processes which are open-loop stable i.e. allows the system to response to disturbances. A striking example of a process with strong inherent control system is the biological system, in which the living organisms are capable of responding, altering and adapting to their environments – e.g. biological robustness (Kitano 2004, Yi, et al. 2000, Barkai and Leibler 1997, Carlson and Doyle 2002).

From this realization, we further propose that the *central goal* of effective partial control design (or external control system) is to augment the inherent control system already possessed by a given process of interest. Therefore, this leads to an idea of *synergistic external-inherent control (SEIC) system* – external control system must work synergistically with the inherent control system. Note that, we refer to the control strategy (e.g. partial control strategy) which is implemented on the process as the *external* control system.

The question is how do we ensure that our control system which we implement on the process will work synergistically with the inherent control capability of a given process of interest? For the time being there is no straightforward answer to this question (so far, there is no research work on this idea). Nevertheless, we propose that the SEIC system can be realized if the nature of the closed-loop and open-loop variables interaction is preserved or at least minimized – thus, related to the second conditions.

Remark 8.1:

Following the idea of SEIC system, it is proposed that the open-loop variables interaction must be maintained by the external control system, thus this leads to similar closed-loop and open-loop variables interaction characteristics. This is the main assumption of SEIC system where an external control system that meets this criterion (or property) is bound to have better performance than those which tend to change the variables interaction characteristics. However, one might ask a question is it possible that the open-loop variables interaction be somehow changed and yet better control performance can still be achieved? To answer this question, it is important that we first clarify what is the measure of 'better control performance' means. Let suppose that the control performance is measured in terms of Integral Square Error (ISE) of the performance measure and the control energy required (i.e.2-norm on manipulated variable signal). Here, ideally we aim to achieve the minimum ISE value with the minimum control energy. Let suppose we compare two control systems, where one achieves SEIC system property and another control system is not i.e. it leads to dissimilar open-loop and closed-loop variables interaction characteristics. From the SEIC system point of view, the first control system should lead to smaller control energy than the second one for a given value of ISE. The reason for this is that, the second control system tends to fight the inherent control system which then tends to lead to larger control energy. In conclusion, any control system which does not possess the SEIC property will be inferior in performance to the one which possesses the SEIC property.

□

In order to test the proposals relating to the two conditions above (Section 8.1.1), we will evaluate and compare the performance of 3 different partial control strategies:

1. CS1: 4x4 control strategy from Chapter 7.
2. CS1-A: 3x3 control strategy with removal of BCL.
3. CS1-B: 3x3 control strategy as in (2) with feedforward control enhancement.

8.2 BCL Impact on CS1 Control Strategy – Preliminary Analysis

Recall in the previous case (Chapter 7), that the dynamic responses of primary controlled variables appear to be quite sluggish. This also leads to a rather slow recovery of the performance measures, which are closely related to these primary (dominant) variables. Initially, we may tend to suspect that the reason for this sluggishness is due to the sluggishness of the inventory control (F_o - L_I loop) i.e. slow movement of F_o leads to slow disturbance especially to the second bioreactor.

Consequently, if this expectation is true then to increase the speed of inventory control and hence the overall control system responsiveness, we can increase the controller gain K_{C1} . However, as shown in Figure 8-1, an increase in K_{C1} from 400 to 500 and even up to 600 has very little effect on the dynamic responses of the output variables. *The question is why such a large increase in K_{C1} has virtually no effect on the dynamic responses?*

It appears that there exists a control-loop which limits the speed of the dynamic responses of variables such that the increase in K_{C1} will not be able to increase the speed of the dynamic responses. This observation suggests the presence of *bottleneck control-loop* (BCL) in the control system.

As the increase in K_{C1} has virtually no effect on the dynamic responses (Figure 8-1), we can conclude that F_o - L_I control-loop (G_{C1}) is unlikely to be the BCL. Next, we can try to alter the controller gain of other control-loop such as the F_I - rx_2 control-loop (G_{C4}) and find out whether this change has any effect on the speed of dynamic responses.

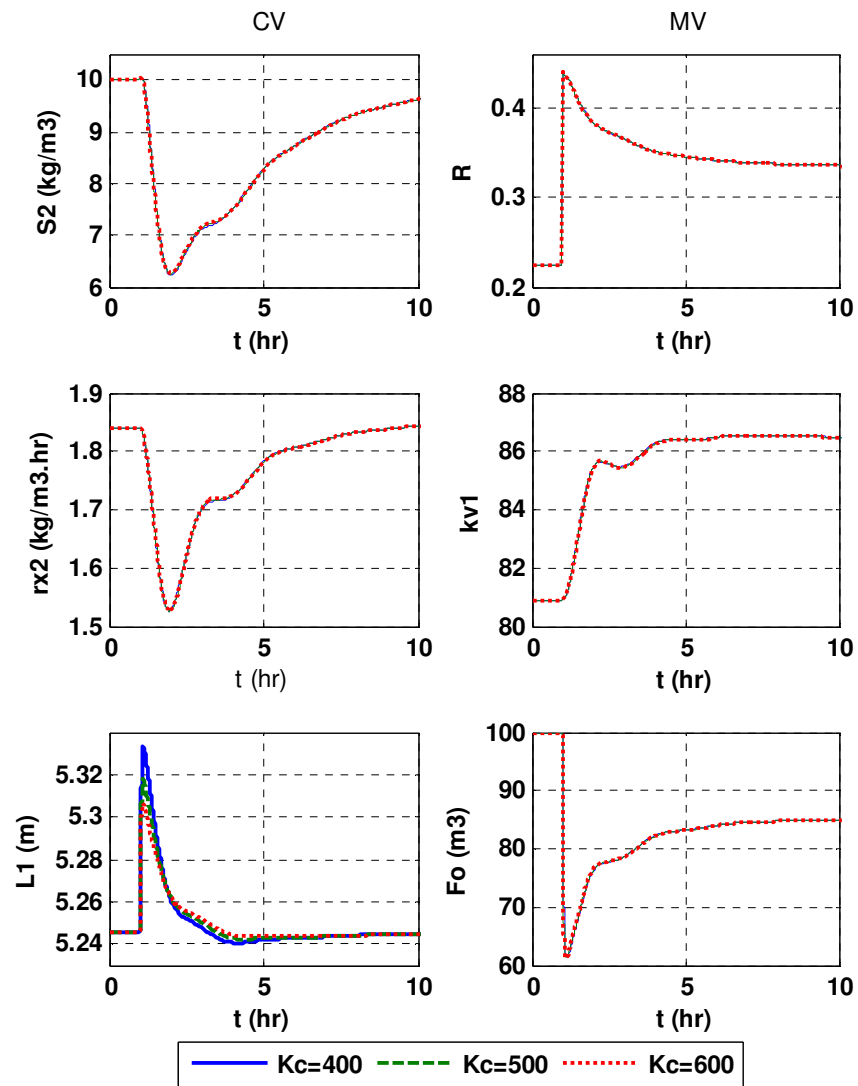


Figure 8-1: Impact of increasing controller gain (K_{c1}) of F_o - L_1 control-loop (G_{c1}) on the dynamic response of control system.

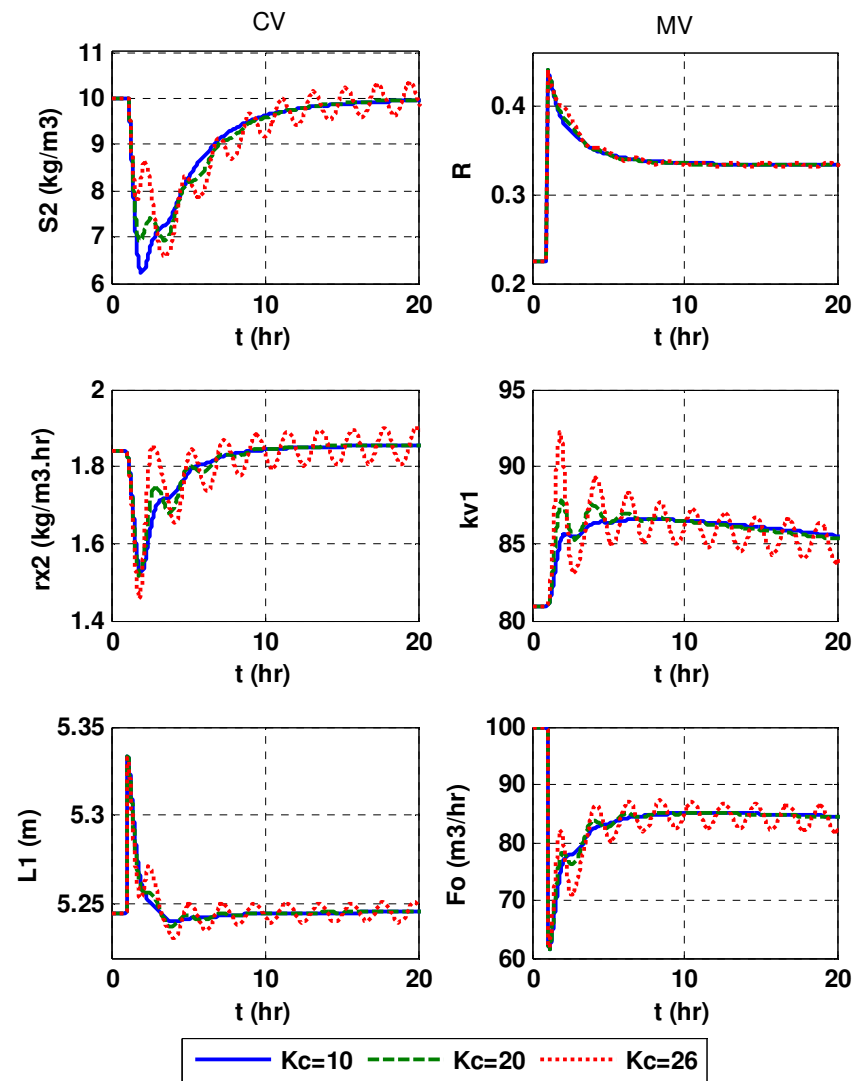


Figure 8-2: Impact of increasing controller gain (K_{c4}) of K_{V_1} - rx_2 control-loop on dynamic responses of S_2 , rx_2 , L_1 , R , kv_1 and F_o

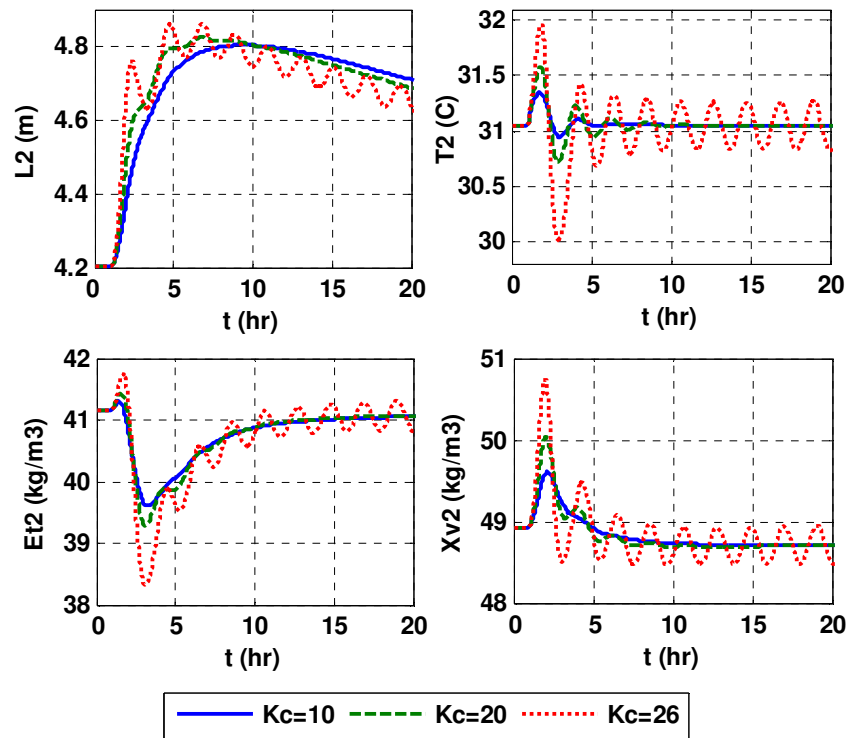


Figure 8-3: Impact of increasing of controller gain K_{c4} (K_{v1-rx_2}) on dynamic responses of L_2 , T_2 , Et_2 and Xv_2

Figures 8-2 and 8-3 show the effect of increasing the controller gain of F_1-rx_2 control-loop (K_{c4}) on the dynamic responses of both controlled and uncontrolled variables. As the controller gain increases, the dynamic responses go from sluggish to oscillatory and to ringing. Figure 8-2 also shows that the responses of the manipulated variables (R , kv_1 and F_o). Notice that, the responses of kv_1 (i.e. F_1) and F_o are also ringing as the controller gain K_{c4} increases from 10 to 26. However, the response of R is almost unaffected by the increase in K_{c4} .

Figure 8-3 shows the dynamic responses of uncontrolled variables: L_2 , Et_2 and Xv_2 as K_{c4} increases. Here, it is important to note that, the response of T_2 (controlled constraint variable) is fluctuating heavily when $K_{c4} = 26$. Thus, this is not desirable because large fluctuation in bioreactor temperature can lead to the degradation in cells performance i.e. biological activity can be adversely affected.

Note that, in this case the increase in K_{c4} fails to significantly improve the speed of responses of all variables (controlled and uncontrolled) and performance measures (not

shown). Rather than improving the speed of dynamic responses, the increase in Kc_4 tends to adversely change the dynamic responses i.e. ringing responses. As such we are expecting that F_I-rx_2 (Gc_4) is the likely candidate for BCL in this control system. Nonetheless, we still need to perform more rigorous analysis (next section) in order to confirm this expectation.

8.2.1 Block Diagram of CS1 Control Strategy

Let Y_{uc1} be the vector of uncontrolled output variables from Sys1 (bioreactor 1) and Y_{uc2} be the vector of uncontrolled output variables from Sys2 (bioreactor 2).

$$Y_{uc1} = \begin{bmatrix} Xv_1 \\ S_1 \\ Et_1 \\ T_1 \end{bmatrix}; \quad Y_{uc2} = \begin{bmatrix} Xv_2 \\ Et_2 \\ T_2 \\ L_2 \end{bmatrix}$$

The following notations are used for the 4 controllers:

- a) $Gc_1 - Fo-L_I$ control-loop
- b) $Gc_2 - R-S_2$ control-loop
- c) $Gc_3 - Fv-T_2$ control-loop
- d) $Gc_4 - F_I-rx_2$ control-loop

Notice that, all of the manipulated variables except for F_I affect the Sys1 (bioreactor 1) first before indirectly affecting Sys2 (bioreactor 2) via the output variables of Sys1. In other words, F_I directly affects Sys1 and Sys2 (see Figure 8-4). Based on Figure 8-4, the “individual unit” process parameters (i.e. rates of growth, substrate consumption and product formation) are assumed to affect the individual system state variables e.g. rx_I , rs_I and rp_I affects directly the state variables of the bioreactor 1.

8.2.2 F_I-rx_2 Control-Loop: Potential BCL in CS1 Control Strategy

From the previous preliminary analysis, the BCL could be the F_I-rx_2 (or Gc_4) due to the nature of slow dynamic response of rx_2 . Consequently, this also leads to slow change in the manipulated variable F_I which in turn becomes slow disturbance to other control loops especially to Gc_1 i.e. notice that from Figure 8-4, F_I has the most direct effect on L_I . As a result, the dynamic response of Gc_1 is always limited by Gc_4 . Subsequently, an

increase in the tuning of G_{c1} cannot really improve the dynamic response of the limiting control-loop. This is the reason why an increase in K_{c1} (in the previous section) has virtually no effect on the speed of dynamic responses as shown previously in Figure 8-1. On the other hand, the increase in the tuning (K_{c4}) of G_{c4} tends to cause oscillatory (even ringing) responses rather than to improve the speed of dynamic responses (see Figures 8-2 and 8-3). Obviously, increasing the tuning values is not the choice for improving the dynamic responses in this case. A better choice is to remove the BCL (possibly G_{c4}) from the control system design, which means that we need to reduce the number of control-loops from four to three i.e. reducing the size of control system to 3x3.

An important question is, to what extent this removal affects (possibly degrade) the speed of dynamic responses and ultimately the performance measures? In other words, the improvement in dynamic performance must outweigh the possible degradation in the overall performance measures, in term of their steady-state variations. Therefore, there must be a trade-off between the improvement of dynamic responses and the steady-state performance specifications.

8.2.3 Direct Feedthrough across Two Bioreactors in CS1 Control Strategy

Notice that from Figure 8-4, the F_1-rx_2 control-loop introduces a direct *feedthrough* of F_1 across bioreactor 1 and bioreactor 2. In this case note that, direct feedthrough is defined as the input which directly affects both system in series. It is expected that the use of this direct feedthrough as a manipulated variable in the CS1 is responsible for altering the open-loop variables interaction; the variables interaction of the closed-loop system is difference from that of the open-loop. As such, from the second condition perspective the CS1 control strategy does not work synergistically with the inherent control system of the TSCE alcoholic fermentation process.

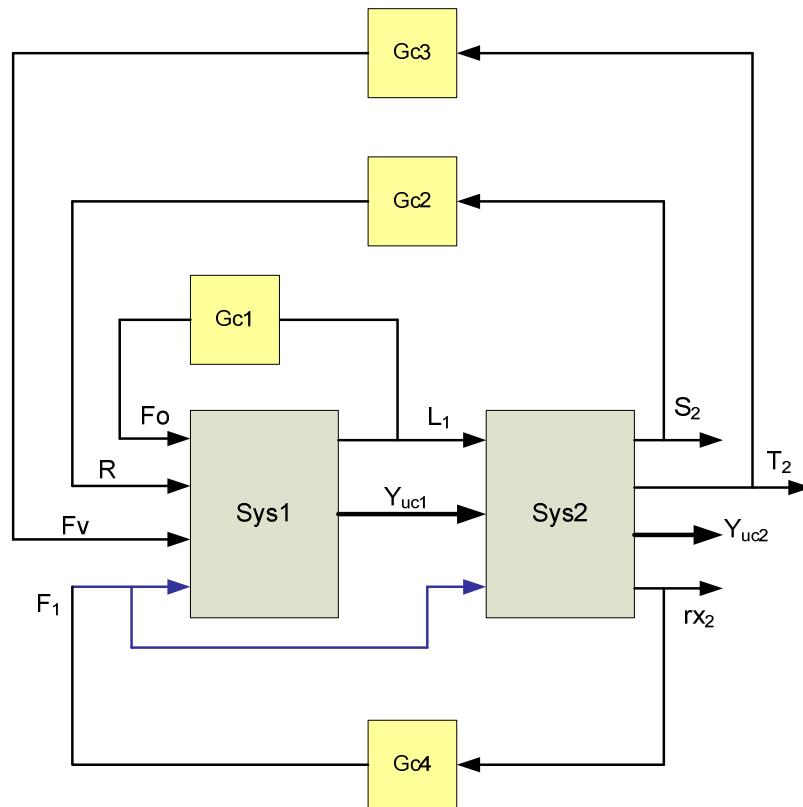


Figure 8-4: Block diagram of 4x4 MIMO control structure

In conclusion, the CS1 control strategy suffers from two main limitations causing it to operate under optimal performance:

1. Potential existence of BCL in the control strategy.
2. The control strategy does not preserve the open-loop variables interaction – external control system does not work in synergy with the inherent control system of the process.

8.3 Analytical Tool for Feedback Control Performance

8.3.1 Singular Value Decomposition (SVD) Concept

Theorem 1: Let $A \in \mathbb{F}^{m \times n}$. There exist unitary matrices

$$U = [u_1, u_2, \dots, u_m] \in \mathbb{F}^{m \times m}$$

$$V = [v_1, v_2, \dots, v_n] \in \mathbb{F}^{n \times n}$$

Such that,

$$A = U\Sigma V^*, \quad \Sigma = \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix}$$

And where the singular values

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p \geq 0, \quad p = \min\{m, n\}$$

The proof for this theorem can be found in (Zhou and Doyle 1998). Note that, the maximum singular value σ_1 is normally denoted as $\bar{\sigma}$ and the minimum singular value as $\underline{\sigma}$.

8.3.2 Feedback Control Performance

Referring to Figure 8-5, the input loop transfer matrix, L_i and output loop transfer matrix, L_o are as:

$$L_i = KP \tag{8-1}$$

$$L_o = PK \tag{8-2}$$

The input sensitivity matrix is defined as transfer matrix from d_i to u_p :

$$S_i = (I + L_i)^{-1} \tag{8-3}$$

$$u_p = S_i d_i \tag{8-4}$$

The output sensitivity matrix is defined as the transfer matrix from d to y :

$$S_o = (I + L_o)^{-1} \tag{8-5}$$

$$y = S_o d \tag{8-6}$$

Meanwhile the input and output complementary sensitivity matrices (i.e. T_i and T_o respectively) are defined as:

$$T_i = I - S_i = L_i(I + L_i)^{-1} \quad 8-7$$

$$T_o = I - S_o = L_o(I + L_o)^{-1} \quad 8-8$$

When the closed-loop system is internally stable, it satisfies the following equations:

$$y = T_o(r - n) + S_o P d_i + S_o d \quad 8-9$$

$$r - y = S_o(r - d) + T_o n - S_o P d_i \quad 8-10$$

$$u = K S_o(r - n) - K S_o d - T_i d_i \quad 8-11$$

$$u_p = K S_o(r - n) - K S_o d + S_i d_i \quad 8-12$$

Thus for good disturbance rejection at the plant output d on the y would require that:

$$\bar{\sigma}(S_o) = 1/\underline{\sigma}(I + PK) \ll 1 \Leftrightarrow \underline{\sigma}(PK) \gg 1 \quad 8-13$$

And good disturbance rejection at the plant input d_i on u_p would require that

$$\bar{\sigma}(S_i) = 1/\underline{\sigma}(I + KP) \ll 1 \Leftrightarrow \underline{\sigma}(KP) \gg 1 \quad 8-14$$

In general, good performance at low frequency range $(0, \omega_l)$ requires:

$$\underline{\sigma}(PK) \gg 1, \underline{\sigma}(KP) \gg 1, \underline{\sigma}(K) \gg 1 \quad 8-15$$

And good robustness and good noise rejection require at high frequency range (ω_h, ∞) :

$$\bar{\sigma}(PK) \ll 1, \bar{\sigma}(KP) \ll 1, \bar{\sigma}(K) \leq M \quad 8-16$$

Here, M is a finite positive number which is not too large.

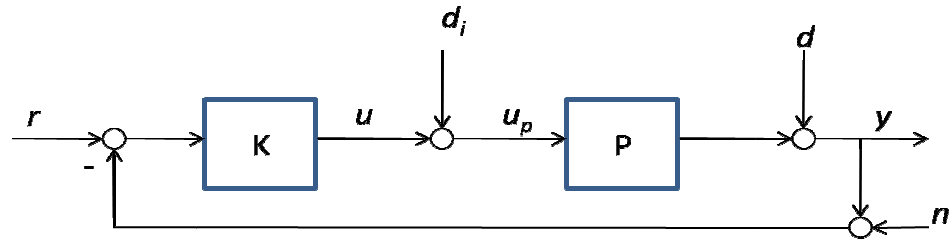


Figure 8-5: Feedback control block diagram (Zhou and Doyle 1998)

8.3.3 Detection of BCL via SVD Analysis

From Eq. 8-14, it is clear that to achieve good performance for disturbance rejection at the plant input, at low frequency range $(0, \omega_l)$ we want to ensure that the $\underline{\sigma}(KP) \gg 1$. Note that, both K and P are square and diagonal, thus $S_o = S_i$. If BCL presents in the control system, then the minimum singular value of KP is expected to be much lower than unity.

Accordingly, the *bottleneck control loop* (BCL) exists in the control system (K) if and only if:

$$\underline{\sigma}(KP) \ll 1 \quad 8-17$$

for a low frequency range $(0, \omega_l)$.

8.4 SVD Analysis of BCL

Note that, the controlled and manipulated variables for the 4x4 control strategy of CS1 is given by:

$$Y_{CV} = \begin{bmatrix} L_1 \\ S_2 \\ T_2 \\ rx_2 \end{bmatrix}, \quad U_{MV} = \begin{bmatrix} F_o \\ R \\ F_v \\ kv_1 \end{bmatrix}$$

Decentralized control strategy (CS1) for 4x4 MIMO control is as follows:

$$K = \begin{bmatrix} Gc_1 & 0 & 0 & 0 \\ 0 & Gc_2 & 0 & 0 \\ 0 & 0 & Gc_3 & 0 \\ 0 & 0 & 0 & Gc_4 \end{bmatrix}$$

The controllers transfer functions are given by:

$$Gc_1 = L_1/F_0 = 120; \quad Gc_2 = S_2/R = \frac{-1.33 \times 10^{-4}(s+0.37)}{s}$$

$$Gc_3 = T_2/F_v = -4; \quad Gc_4 = rx_2/F_1 = \frac{13(s+0.85)}{s}$$

Meanwhile for the 3x3 (F_I - rx_2 control-loop removed) control system, the P or PI controller tunings are given by

$$Gc_1 = \frac{400(s+0.9)}{s}; \quad Gc_2 = \frac{-4.428 \times 10^{-4}(s+0.67)}{s}; \quad Gc_3 = -4$$

Note that, in the 3x3 decentralized control strategy, the BCL which is Gc_4 is eliminated – thus, no direct control of growth rate in bioreactor 2.

8.4.1 Linear Transfer Function Models

The linear transfer functions matrix for 4x4 MIMO plant obtained at the nominal operating conditions is given by:

$$P = \begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} \\ g_{21} & g_{22} & g_{23} & g_{24} \\ g_{31} & g_{32} & g_{33} & g_{34} \\ g_{41} & g_{42} & g_{43} & g_{44} \end{bmatrix}$$

Where the linearized models are given by:

$$g_{11} = \frac{0.051(s+0.918)(s+0.383)(s+0.0007)(s^2+3.444s+3.749)}{(s+1.173)(s+0.465)(s+0.257)(s+0.001)(s^2+3.501s+4.019)}$$

$$g_{21} = \frac{0.108(s+17.22)(s-0.184)(s-0.0003)(s^2+1.905s+10.39)}{(s+0.469)(s+0.003)(s^2+1.457s+1.452)(s^2+5.69s+17.62)}$$

$$g_{31} = \frac{-0.01(s-76.4)(s^2+0.026s+0.0002)(s^2+1.467s+2.81)(s^2+5.55s+11)}{(s+4.7)(s+0.623)(s+0.0009)(s^2+1.36s+2.97)(s^2+4.48s+9.58)}$$

$$g_{41} = \frac{0.004(s+16.1)(s-12.3)(s-0.0006)(s^2+1.73s+1.26)}{(s+1.39)(s+0.002)(s^2+1.23s+1.54)(s^2+4.99s+12.6)}$$

$$g_{12} = \frac{10.2(s+0.805)(s+0.095)(s^2+4.38s+5.1)}{(s+1.15)(s+0.301)(s+0.091)(s^2+4.41s+5.3)}$$

$$g_{22} = \frac{-6.94(s+0.002)(s^2+2.48s+2.55)(s^2-14.8s+128.6)}{(s+0.5)(s+0.0001)(s^2+1.81s+1.85)(s^2+6.45s+18.2)}$$

$$g_{32} = \frac{0.041(s+2988)(s^2-0.001s+2.3 \times 10^{-5})(s^2+5.2s+12.5)}{(s+2.41)(s+1.1)(s+0.29)(s+3.5 \times 10^{-5})(s^2+4.99s+12.3)}$$

$$g_{42} = \frac{-0.154(s+93.9)(s-0.011)(s-0.005)(s^2+13.3s+54.4)}{(s+6.55)(s+0.81)(s^2+0.0008s+0.0001)(s^2+4.8s+10.8)}$$

$$g_{13} = \frac{-0.014(s+0.659)(s+0.236)(s-0.0006)(s^2+5.81s+9.57)}{(s+1.186)(s+0.377)(s+0.075)(s+10^{-5})(s^2+5.74s+9.5)}$$

$$\begin{aligned}
g_{23} &= \frac{0.045(s+1.61)(s+0.15)(s+0.005)(s^2-5.69s+317.8)}{(s+3.8)(s+2.16)(s+1)(s+0.86)(s+0.072)(s+0.003)} \\
g_{33} &= \frac{0.001(s-2006)(s+3.91)(s+0.916)(s+0.066)(s-0.003)}{(s+3.76)(s+2.342)(s+0.057)(s+0.0001)(s^2+1.68s+0.72)} \\
g_{43} &= \frac{-0.0002(s-1053)(s+6.827)(s+1.437)(s+0.093)(s+0.0007)}{(s+3.798)(s+2.399)(s+1.032)(s+0.843)(s+0.093)(s+0.0001)} \\
g_{14} &= \frac{-0.093(s+3.973)(s+2.505)(s-0.0006)(s^2+0.782s+0.166)}{(s+4.232)(s+2.06)(s+1.517)(s+0.0015)(s^2+0.658s+0.124)} \\
g_{24} &= \frac{0.827(s+0.005)(s^2-0.232s+3.412)(s^2+7.502s+56.47)}{(s+3.465)(s+0.017)(s^2+2.2s+1.799)(s^2+8.534s+43.35)} \\
g_{34} &= \frac{0.682(s+11.09)(s+5.321)(s-0.974)(s+0.058)(s-0.002)}{(s+10.78)(s+7.054)(s+2.312)(s+0.412)(s+0.0001)} \\
g_{44} &= \frac{-0.158(s+17.52)(s-0.942)(s+0.043)(s^2+1.231s+1.161)}{(s+2.095)(s+0.054)(s^2+0.918s+0.877)(s^2+14.14s+53.11)}
\end{aligned}$$

Note that, the models are obtained through a series of plant step tests: F_o , F_I , R and F_v as inputs (manipulated variables) and S_2 , rx_2 , T_2 and T_2 as recorded outputs. Then the model identification is performed using the Matlab System Identification toolbox. The size of the step input perturbation for each manipulated variable is 20% of its nominal value (refer to Chapter 5, Section 5.4 for the nominal values of R , r , F_o) and F_v nominal value is $1.0 \text{ m}^3/\text{hr.}$.

Remark 8.2:

The magnitude of inputs change for the plant tests are 20% of their nominal values. Here, the objective of the linear models development is to approximate the linear dynamics around the nominal operating conditions. Alternatively, direct linearization of the system at the nominal operating conditions can also lead to the linear representation of the dynamic behaviour. In this case, we choose to develop the linearized models from the step tests because the direct linearization tends to lead to unstable models (large model error at the optimum, which is not consistent with the nonlinear model prediction at the nominal operating conditions i.e. response based on the actual nonlinear model is stable.

□

8.4.2 SVD Analysis of CS1 Control Strategy

Recall that from Section 8.5, we are interested in the minimum singular value of KP where it is desirable that $\underline{\sigma}(KP) \gg 1$. Otherwise, if $\underline{\sigma}(KP) \ll 1$ there is bound to be a BCL in the control system.

As can be seen from Figure 8-6, the minimum singular value at low frequency is much less than 1, i.e. $\underline{\sigma}(KP) \ll 1$. Thus, this indicates the present of BCL in the control system K for CS1 strategy. In other words, one of the control-loops is limiting the performance of the overall control system. *What happen if we increase the controller gain of the suspected BCL which is the G_{c4} ? Can the increase in K_{c4} leads to the increase in the minimum singular value?*

Figure 8-7 displays the singular values plot for $K_{c4} = 26$ i.e. double the previous value of K_{c4} . Obviously from Figure 8-7, doubling the controller gain K_{c4} does not have any significant impact on the minimum singular value, i.e. it is still very low. This result confirms the previous analysis why an increase in K_{c4} fails to increase the speed of dynamic response. No change in the minimum singular value implies that there will be no change in the speed of the dynamic responses.

Now, let change the other controller gain such as the K_{c1} (G_{c1} which controls the liquid level in bioreactor 1). Figure 8-8 shows the impact of increasing the K_{c1} from 120 to 300. The singular values plot marginally changes but the minimum singular value at low frequency remains very low. Hence, this suggests that the speed of BCL (i.e. thus the speed of the overall dynamic responses) cannot really be increased by increasing the gain of other control-loop (consistent with the result shown in Figure 8-1).

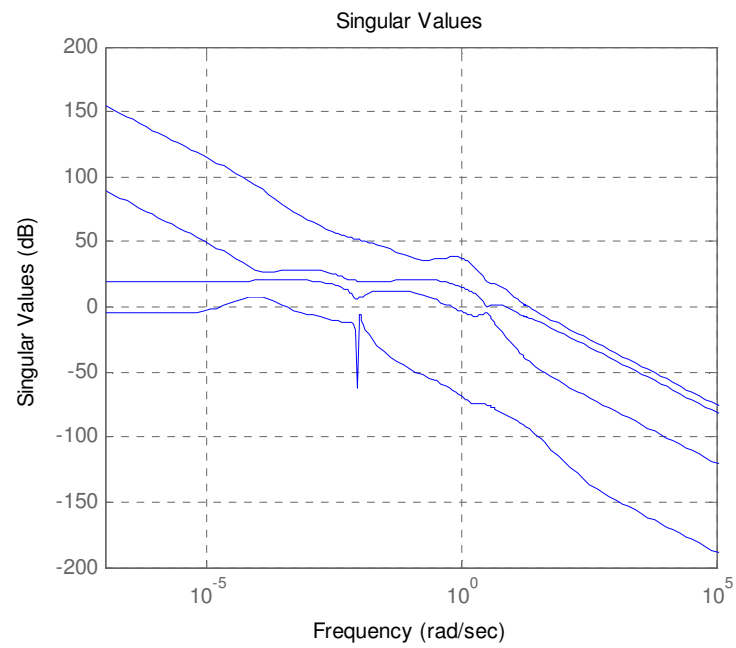


Figure 8-6: Singular values of KP for $K_{c4} = 13$

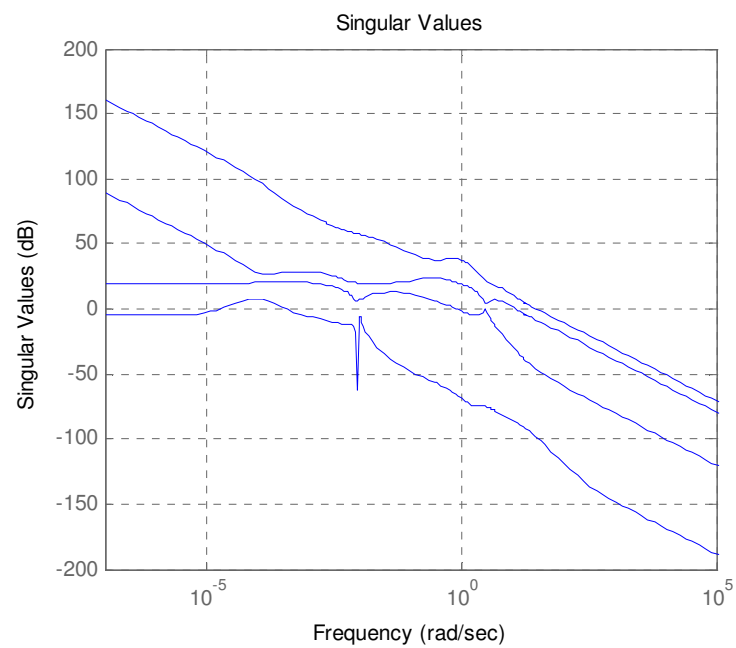


Figure 8-7: Singular values plot of KP with $K_{c4} = 26$

8.4.3 SVD Analysis of 3x3 (CS1-A) Control Strategy

Figure 8-9 shows the singular values plot for the 3x3 (CS1-A) control system where the G_{c4} is removed from the CS1 control strategy. Notice that, the minimum singular value at low frequency range is now much larger (above 1) than in the case of 4x4 (CS1) control strategy. Therefore, this confirms that BCL has been removed from the control system. Hence in this case, the BCL is confirmed to be the F_{I-rx2} control-loop i.e. G_{c4} .

We can draw a conclusion from the singular values plot that 3x3 system will be more responsive (because its $\underline{\sigma} \gg 1$) than that of 4x4 system because in the latter the performance is limited by the presence of BCL (i.e. its $\underline{\sigma} \ll 1$).

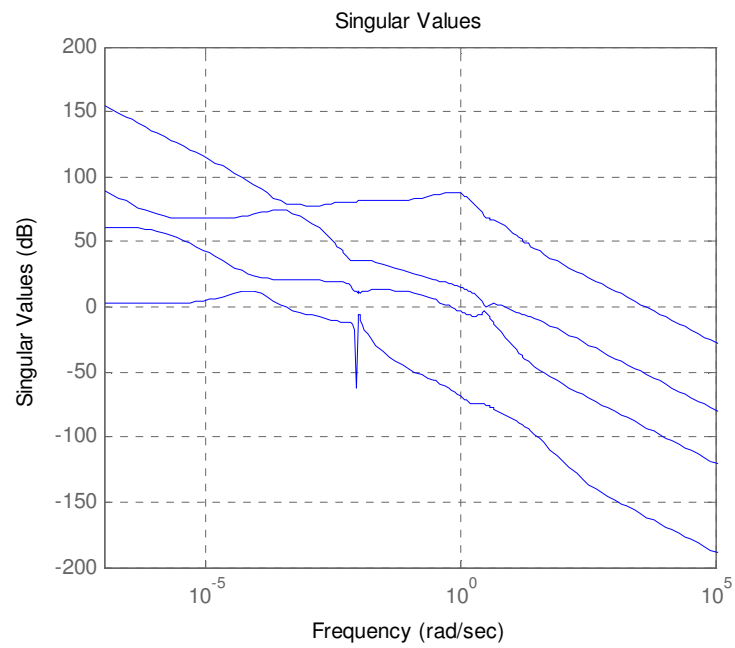


Figure 8-8: Singular values plot of CS1 for KP with $K_{c1} = 300$

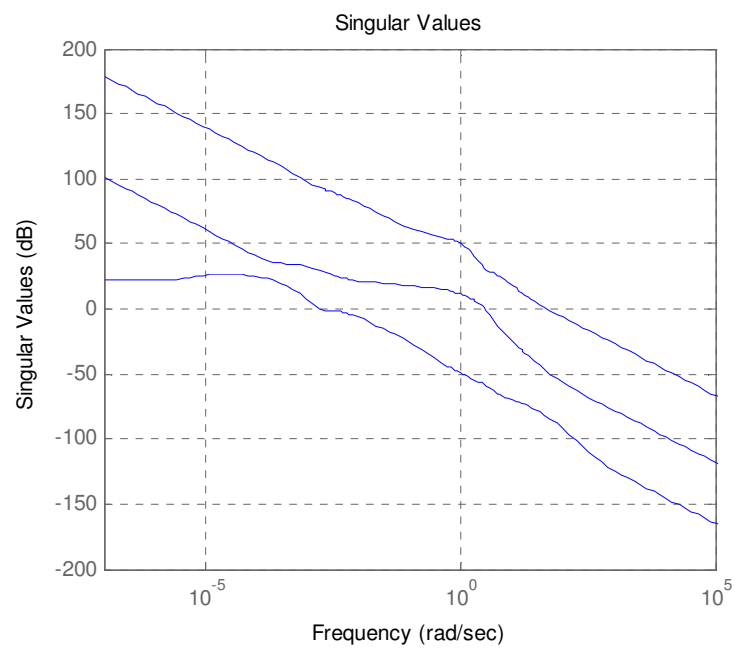


Figure 8-9: Singular values plot of CS1-A for KP i.e. 3x3 control system

8.5 Comparative Performances of Different Partial Control Strategies: CS1, CS1-A and CS1-B

The performance of the following 3 partial control strategies are evaluated and compared against the step disturbance in fresh substrate concentration (S_o):

- i. CS1: (4x4 MIMO) with feedforward enhancement (Chapter 7)
- ii. CS1-A: (3x3 MIMO) with removal of BCL
- iii. CS1-B: (3x3 MIMO) with feedforward control enhancement.

Figures 8-10 and 8-11 display the schematics of 3x3 control strategies without and with feedforward enhancement (i.e. CS1-A and CS1-B) respectively. The schematic of CS1 is shown in the previous Chapter 7. Note that, the feedforward controllers employed in CS1 and CS1-B are identical i.e. similar in terms of structure and tuning values. Note that, this feedforward controller is designed based on the first order approximations (models) of the impact of cell recycle ratio (R) and fresh substrate concentration (S_o) on the substrate concentration in bioreactor 2 (S_2). The dynamic responses which are used to develop the first order approximations, and hence which are used to derive the feedforward controller can be referred Figure 7-8, Chapter 7. The step change in the manipulated variable (R) is 0.05 and the step change in disturbance (S_o) is 30 kg/m^3 .

The reason why the feedforward controller used in CS1-B is similar to that used in CS1 is that in both cases they are derived from the same step responses. In practice, we can perform fine tuning of both feedforward controllers to achieve a desired performance (i.e. optimization of the tuning parameters). However, in our case the tuning parameters are fixed by the linear models derived from the step responses (refer to Figure 7-8, Chapter 7) - no attempt is made to optimize the tuning parameters. Note that, in the 3x3 control strategies (CS1-A and CS1-B), only one of the dominant variable is controlled, which is the substrate concentration in bioreactor 2, i.e. S_2 .

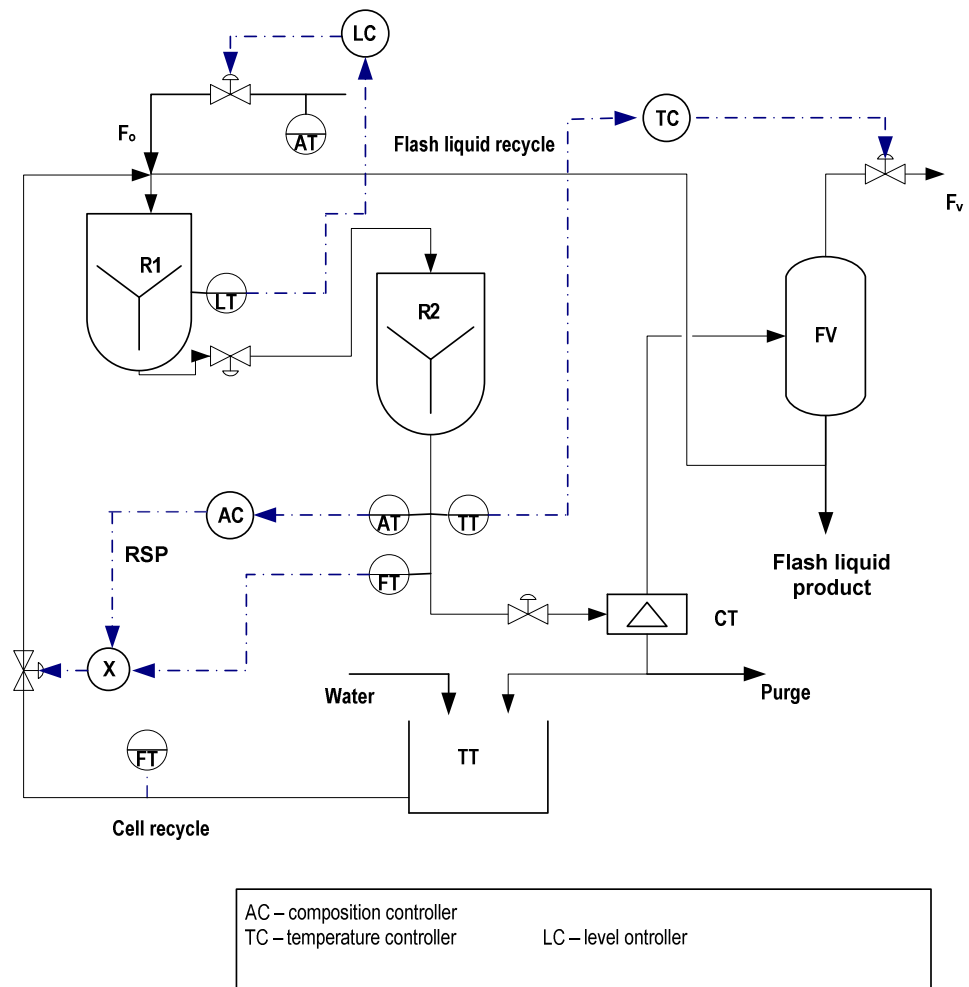


Figure 8-10: 3x3 control strategy (CS1-A) without feedforward enhancement.

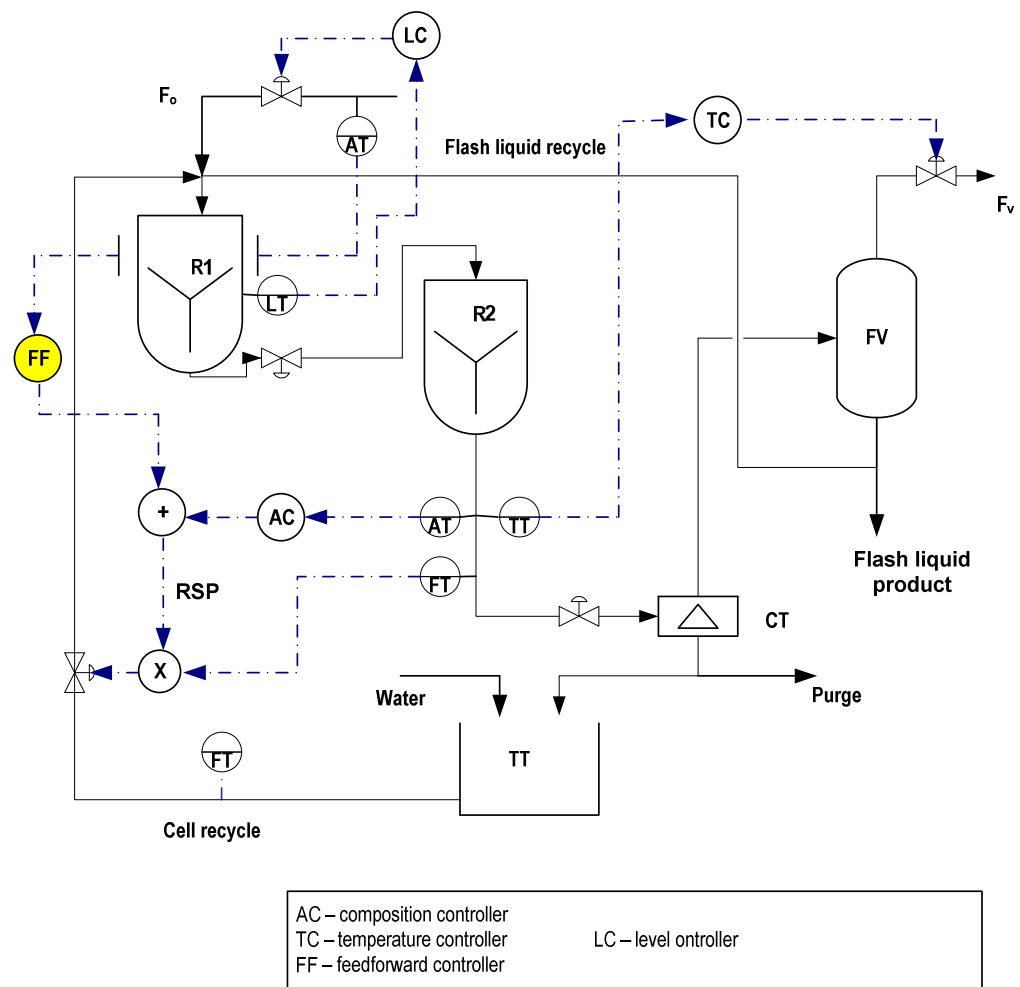


Figure 8-11: 3x3 control strategy augmented with feedforward control (CS1-B)

8.5.1 Impact of Removing BCL: Analysis via I_{DV}

Bear in mind Chapter 6, the values of closeness index (CI) are as tabulated in Table 6-3. Using the values of CI in Table 6-3, we can form a matrix called the dominant variable interaction array I_{DV} as:

$$I_{DV} = \begin{bmatrix} \delta_{1,1} & \delta_{1,2} & \delta_{1,3} \\ \delta_{2,1} & \delta_{2,2} & \delta_{2,3} \\ \delta_{3,1} & \delta_{3,2} & \delta_{3,3} \end{bmatrix} = \begin{bmatrix} 0.002 & 0.019 & 0.083 \\ 0.163 & 0.193 & 0.084 \\ 0.167 & 0.194 & 0.051 \end{bmatrix} \quad 8-18$$

Notice that the values of elements in the 1st row of I_{DV} (i.e. values corresponding to S_2 in the directions of performance measures) are largely small as compared to those in the 2nd row (values corresponding to S_1). Thus, this indicates that S_2 has larger influence than S_1 on the performance measures (*Yield*, *Conv* and *Prod*). To assess whether it is sufficient to control only S_2 , let us invoke the algorithm described in Chapter 4 (Section 4.4.4.5) to analyze the extent of interaction between the dominant variables and performance measures. Also let us specify that $\delta_{max} = 0.09$ for this case i.e. similar threshold value as in the I_{VV} analysis described previously in Chapter 7 (Section 7.2.3).

Inspection of the maximum element in the 1st row corresponding to the most influential dominant variable (S_2) yields:

$$I_{1,max} = \max_{\delta_{1,j}|j=1\dots3} (I_{DV}|_1) = \max(0.002, 0.019, 0.083) = 0.083$$

As $I_{1,max} < 0.09$, then this indicates that it is sufficient to control only S_2 to meet all 3 overall performance measures: we can ensure acceptable variations in performance measures just by controlling only S_2 . Thus, in light of this analysis the basic partial control design mentioned previously in Chapter 6 is “over controlled” in the sense that, there are too many controlled variables to achieve the overall performance measures. It is imperative in the control system design to control the minimum number of variables because this not only can result in lower cost but also can avoid the presence of BCL in the control system. As in this case study, if BCL does presence in the control system (which can be detected via SVA analysis), we must apply judicious analysis (e.g. using I_{DV}) before we decide either to remove or keep the control-loop that is known to be BCL.

If I_{DV} analysis shows that the removal of this BCL will not severely penalize the steady-state performance ($I_{i,max} < \delta_{max}$), then it is justified to reduce the size of the control system by removing the BCL in order to gain better dynamic performance.

8.5.2 Dynamic Simulation Results

8.5.2.1 Disturbance Rejection: Fresh Substrate Concentration ($\Delta S_o = \pm 30 \text{ kg/m}^3$)

Figure 8-12 indicates the dynamic responses of the 3 performance measures when subject to step disturbance in S_o with magnitude of $\pm 30 \text{ kg/m}^3$. For *Yield*, there is no marked dynamic improvement using 3x3 control strategies (either CS1-A or CS1-B) over that of 4x4 control strategy with feedforward enhancement. On the other hand for *Conv*, there is a significant dynamic improvement with CS1-B (3x3 with feedforward enhancement) over that of CS1. Additionally, not only the settling time for *Conv* is fastest under CS1-B but also the peak change during the transient response is the smallest. It is interesting to note that, even without feedforward enhancement, the 3x3 control strategy (CS1-A) exhibits significant improvement in the *Conv* dynamic response over that of CS1 for the case of step increase in S_o . However, no marked improvement in the *Conv* response is made when subject to step decrease in S_o .

An interesting point to note is that, the 3x3 control strategies show the largest improvement in the dynamic response of *Prod*. Even without the feedforward enhancement, the 3x3 control strategy (CS1-A) can achieve significant improvement over that of 4x4 control strategy (CS1). It is rather surprising, however, that for the 3x3 control strategies the dynamic responses of *Prod* are quite comparable with and without the feedforward enhancement. In other words, we can achieve good performance in term of *Prod* with 3x3 control strategy even without the feedforward enhancement – simple strategy that can do the work well.

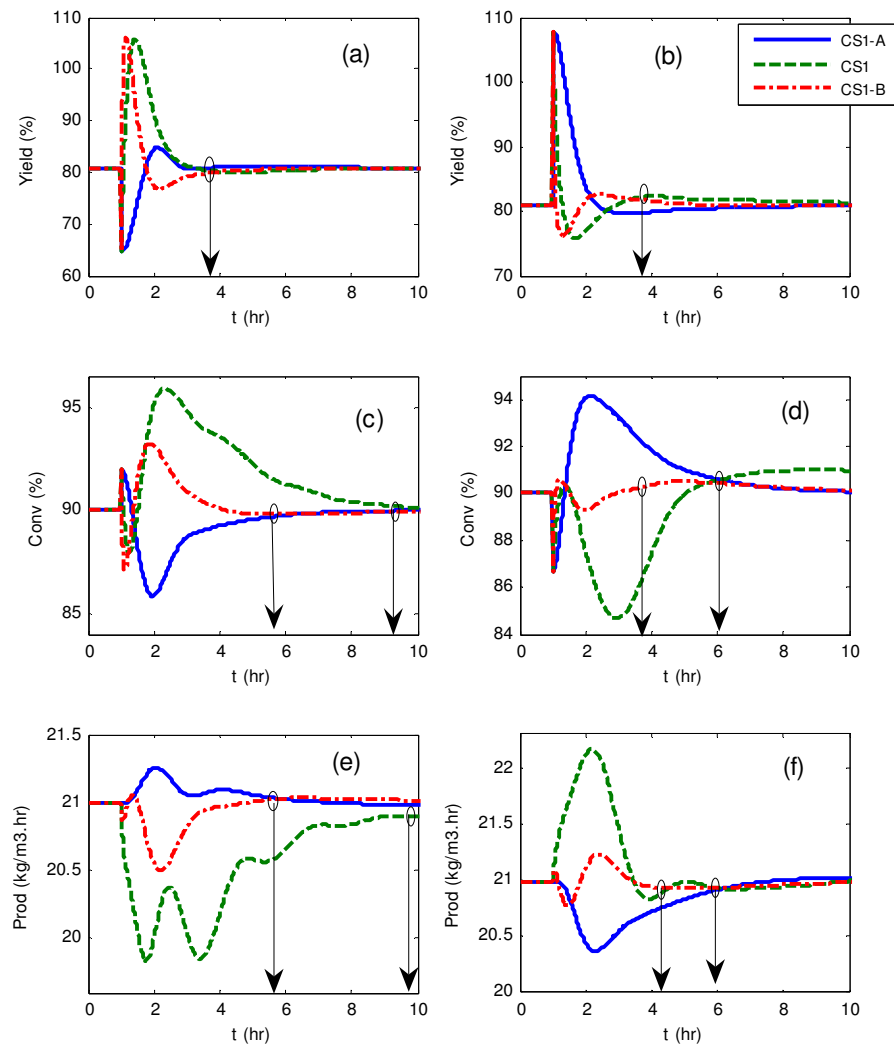


Figure 8-12: Dynamic responses of performance measures (arrows indicate the settling times): magnitude of step disturbance in $S_o = 30 \text{ kg/m}^3$

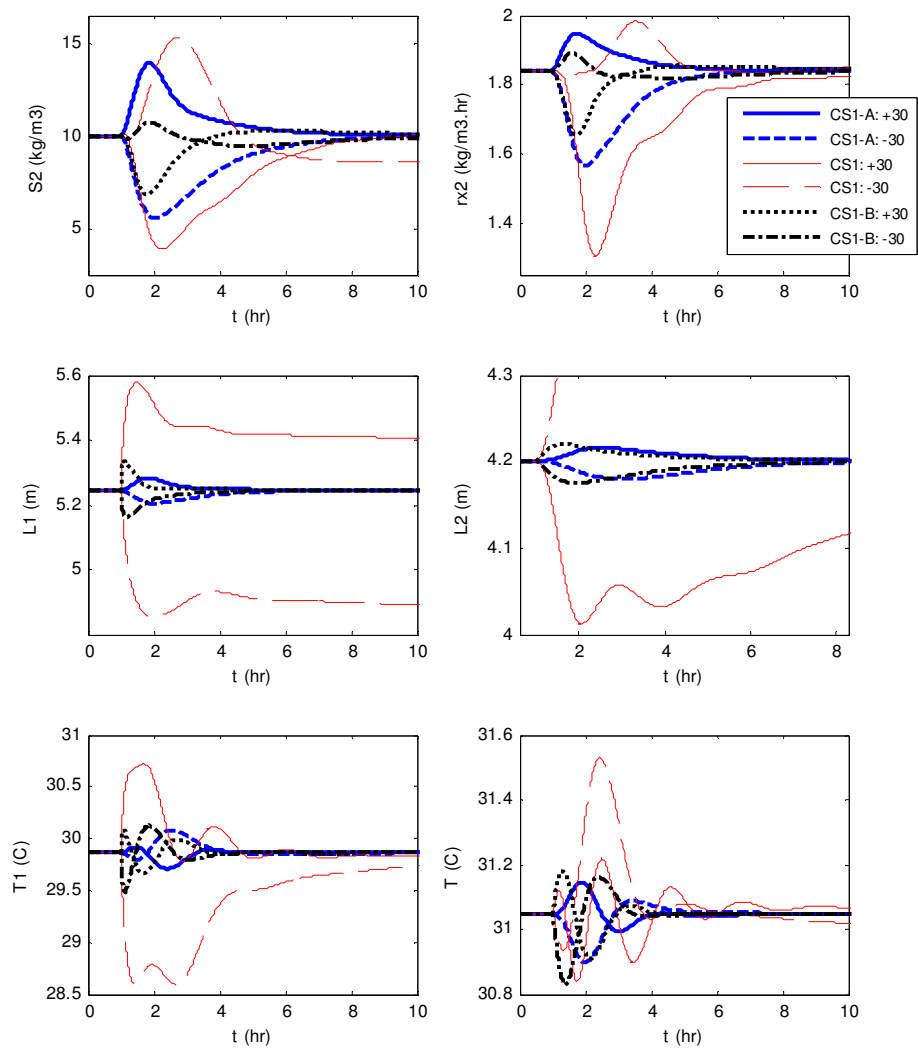


Figure 8-13: Dynamic responses of controlled and uncontrolled variables: magnitude of step disturbance in $S_0 = 30 \text{ kg/m}^3$

Figure 8-13 shows the responses of primary, inventory and constraint variables under different partial control strategies. Overall the dynamic responses of the 3x3 control strategies are better than that of 4x4 control strategy in terms of faster settling time and smaller peak change during the transient period. Notice that, in term of primary variables (S_2 and rx_2) responses, the CS1-B gives the best dynamic performance followed by CS1-A. Also it is important to note that, the dynamic response of rx_2 under CS1-A and CS1-B (3x3 control strategies) are significantly improved over that under the CS1 control strategy.

Hence, this confirms close interaction between S_2 (controlled variable) and rx_2 (uncontrolled variable) as suggested by the dominant variable interaction analysis previously. Another important point to note is that, the steady-state values of S_2 and rx_2 under different control strategies tend to converge to within similar range of values i.e. small offset of rx_2 under CS1-A and CS1-B.

As can be observed from Figure 8-13, large improvement in the dynamic responses of inventory variables (L_1 and L_2) can be achieved with the 3x3 control strategies. Notice from that figure, the peak fluctuations in L_1 and L_2 are very small under CS1-A and CS1-B as compared with the peak fluctuations under CS1. Such an improvement (i.e. reduction) in the inventory variables fluctuations is beneficial because it allows us to operate closer to the maximum bioreactor volume, which in turn improves the economic performance – the closer to maximum volume the better the economic performance. It is interesting to note that for the inventory variables case, CS1-A and CS1-B show very closed dynamic performance i.e. without and with feedforward enhancement show comparable performance.

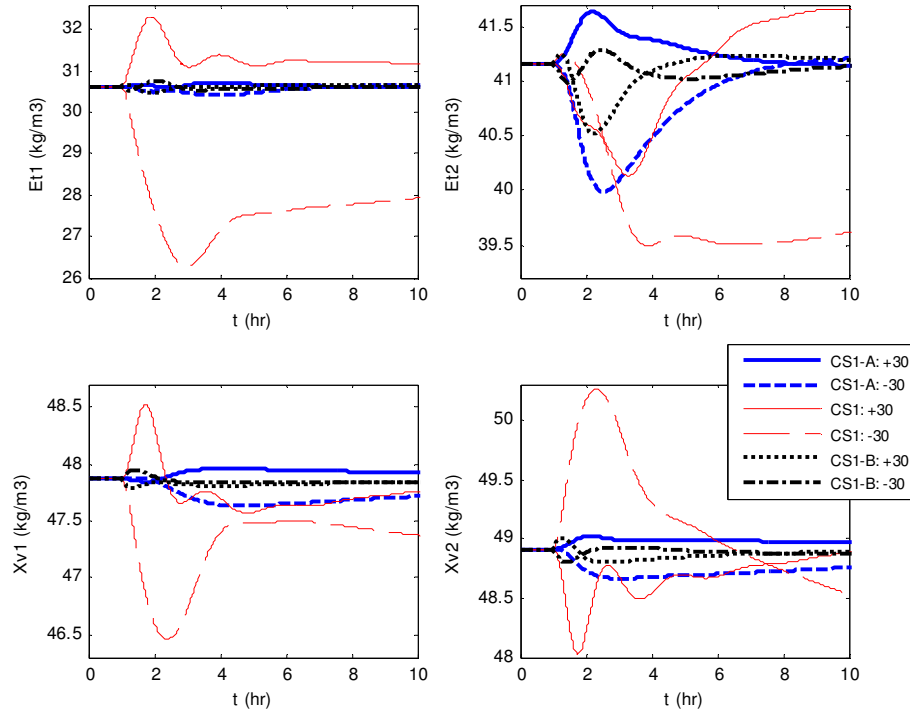


Figure 8-14: Dynamic responses of other uncontrolled variables: magnitude of step disturbance in $S_o = 30 \text{ kg/m}^3$

Just like the inventory variables case, the dynamic responses of constraint variables (T_1 and T_2) also show significant improvement under 3x3 control strategies (peak change is small as compared with that under CS1). In addition, both CS1-A and CS1-B also show comparable performance. Figure 8-14 shows the other uncontrolled variables: Et_1 , Et_2 , Xv_1 and Xv_2 . The result further confirm that the 3x3 control strategies are superior in terms of providing faster speed of response and lower peak change to 4x4 control strategy. Overall, the reduced size partial control strategies (3x3) demonstrates better dynamic performance than the 4x4 control strategy. Also it is interesting to note that, it seems that there is no loss in steady-state performance due to the removal of BCL from the 4x4 control strategy i.e. as expected from the result of assessment using the I_{DV} index (Section 8.5.1).

8.5.2.2 *Disturbance Rejection: Fresh Substrate Concentration ($\Delta S_o = \pm 10 \text{ kg/m}^3$)*

Recall from Chapter 5, the TSCE alcoholic fermentation system is strongly nonlinear. Therefore, the large variation in the disturbance applied in the previous Section 8.5.2.1 is expected to significantly excite the nonlinearity of the system. But despite this large nonlinearity excitation, all of the partial control strategies studied so far have shown stable responses. It is interesting to find out how these control strategies perform against a relatively small disturbance magnitude i.e. change in S_o is only 10 kg/m^3 . In this case, we will compare only CS1 and CS1-A control strategies.

From Figure 8-15, under the CS1 the dynamic responses of S_1 and S_2 are significantly faster (with lower peaks) than those under CS1-A. This result is opposite to the large step change in S_o ($\Delta S_o = \pm 30 \text{ kg/m}^3$) used in the previous section. However, the responses of inventory and constraint variables remain significantly faster under CS1-A than under CS1. For the case of inventory variables, recall that under CS1 when the disturbance magnitude is 30 kg/m^3 , L_1 and L_2 exhibit the opposite dynamic trends (closed-loop variables interaction is different from the open-loop variables interaction). Interestingly when the magnitude of disturbance is only 10 kg/m^3 , L_1 and L_2 show quite similar dynamic trends (i.e. having similar directions as predicted by the open-loop variables interaction) under the CS1 control strategy. However, the degree of interaction between L_1 and L_2 seem to be weaker under the CS1 than their degree of interaction under the CS1-A (i.e. L_2 steady-state offset is quite large under the CS1 as compared with that under the CS1-A).

This result however suggests that, the variables interaction characteristics can not only depend on the control structure but also depend on the operating conditions i.e. extent of nonlinearity excitation due to the disturbance occurrence. Figure 8.16 shows the dynamic responses of the performance measures which are quite comparable under both control strategies. Thus, for small change in disturbance, both control strategies CS1 and CS1-A seems to have almost comparable performance in term of meeting the overall control objective. However, CS1-A shows markedly better performance in terms of meeting the inventory and constraint control objectives.

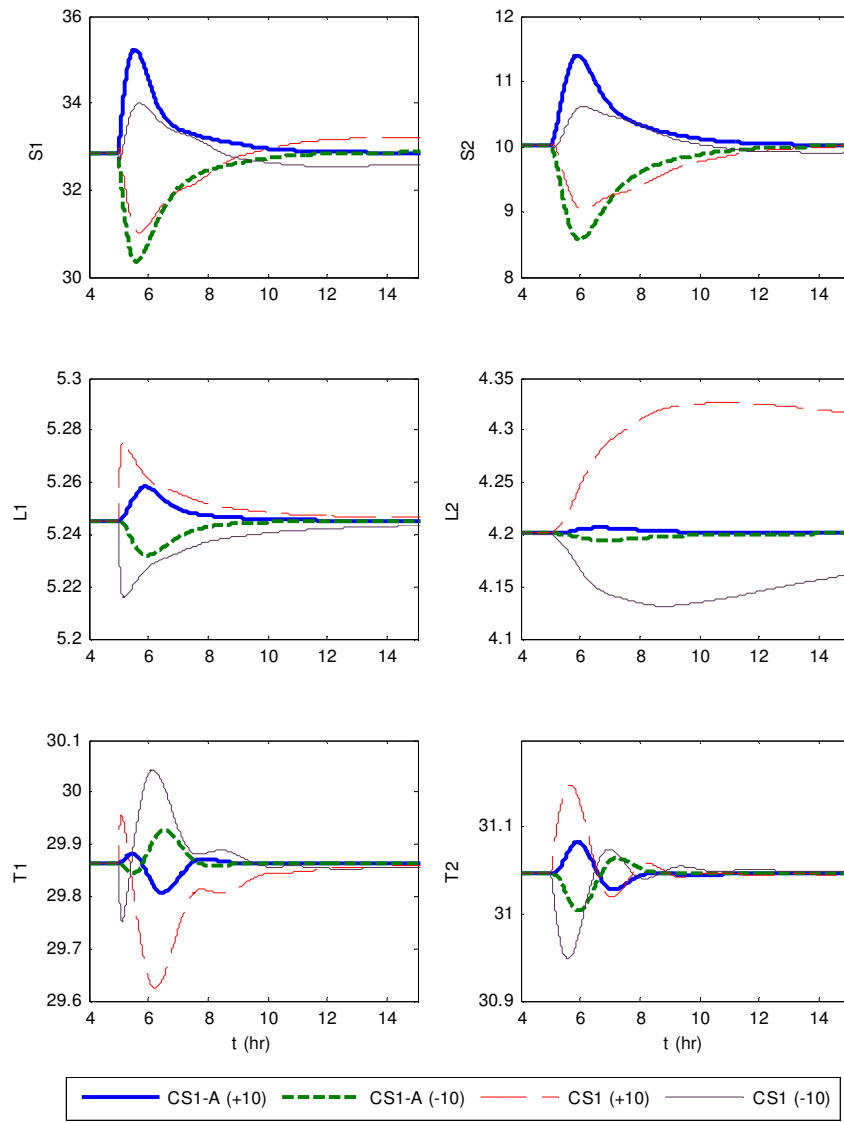


Figure 8-15: Dynamic responses of controlled and uncontrolled variables correspond to $\Delta S_o = \pm 1.0 \text{ kg/m}^3$

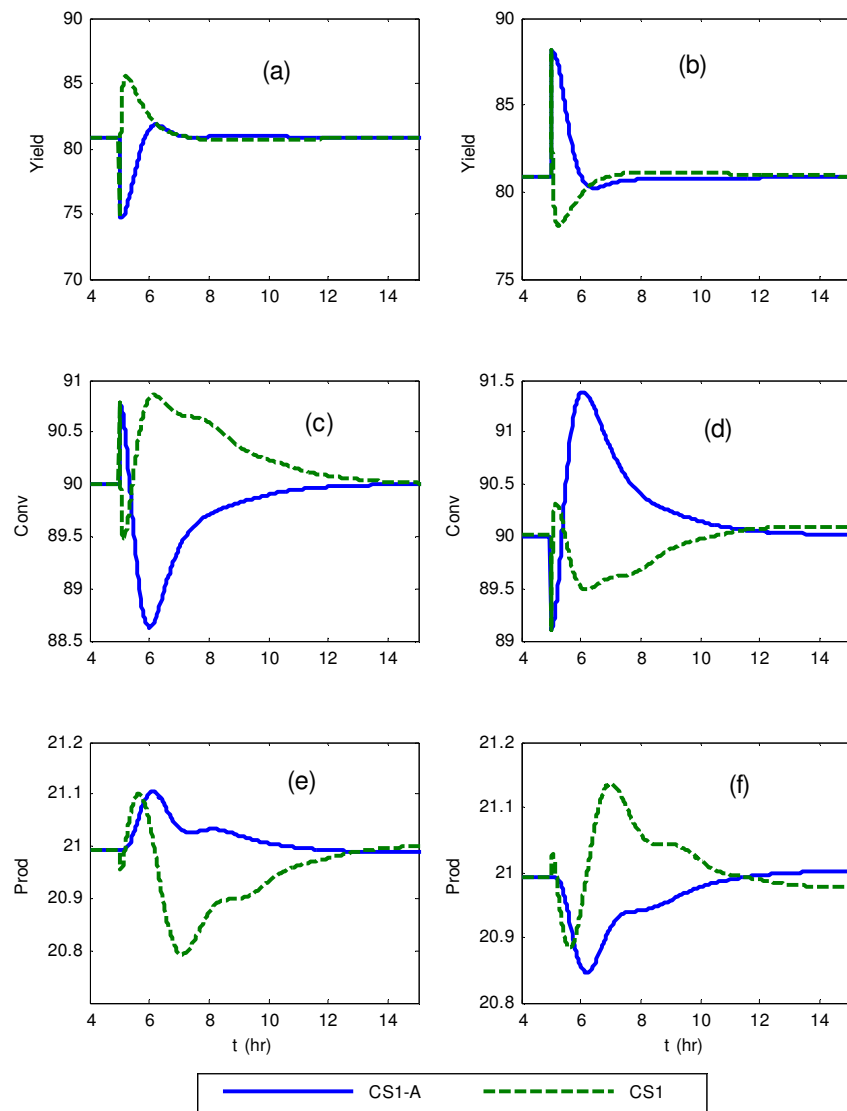


Figure 8-16: Dynamic responses of the performance measures: (a), (c) and (e) correspond to $\Delta S_0 = 10 \text{ kg/m}^3$; (b), (d) and (f) correspond to $\Delta S_0 = -10 \text{ kg/m}^3$

8.5.2.3 *Disturbance Rejection: Fresh Inlet Flow Temperature ($\Delta T_o = 1^\circ\text{C}$)*

Apart from the change in the fresh substrate concentration S_o , another important source of disturbance to the TSCE alcoholic fermentation process is the fluctuation in the temperature of the fresh substrate stream T_o . Therefore, it would be interesting to find out how the different control strategies (CS1 and CS1-A) respond to this temperature disturbance. To test their performance against T_o disturbance, a step change (increase) of 1.0°C in T_o is applied to the TSCE alcoholic fermentation system.

Figure 8-17 shows the dynamic responses of the performance measures and controlled variables (S_2 , T_2 and L_1) against the step increase in T_o by 1.0°C . Note that, the responses of *Yield*, *Conv* and *Prod* are markedly better under the CS1-A than under the CS1. The greatest advantage of the CS1-A strategy over CS1 is the fast dynamic response of inventory variables under the former control strategy; sluggish responses of the inventory variables under the CS1. Notice also that there is a significant offset in the constraint variables as the temperature control only employs P-only controller. It is important to note that, we can remove the temperature offset by employing PI controller instead of P-only controller.

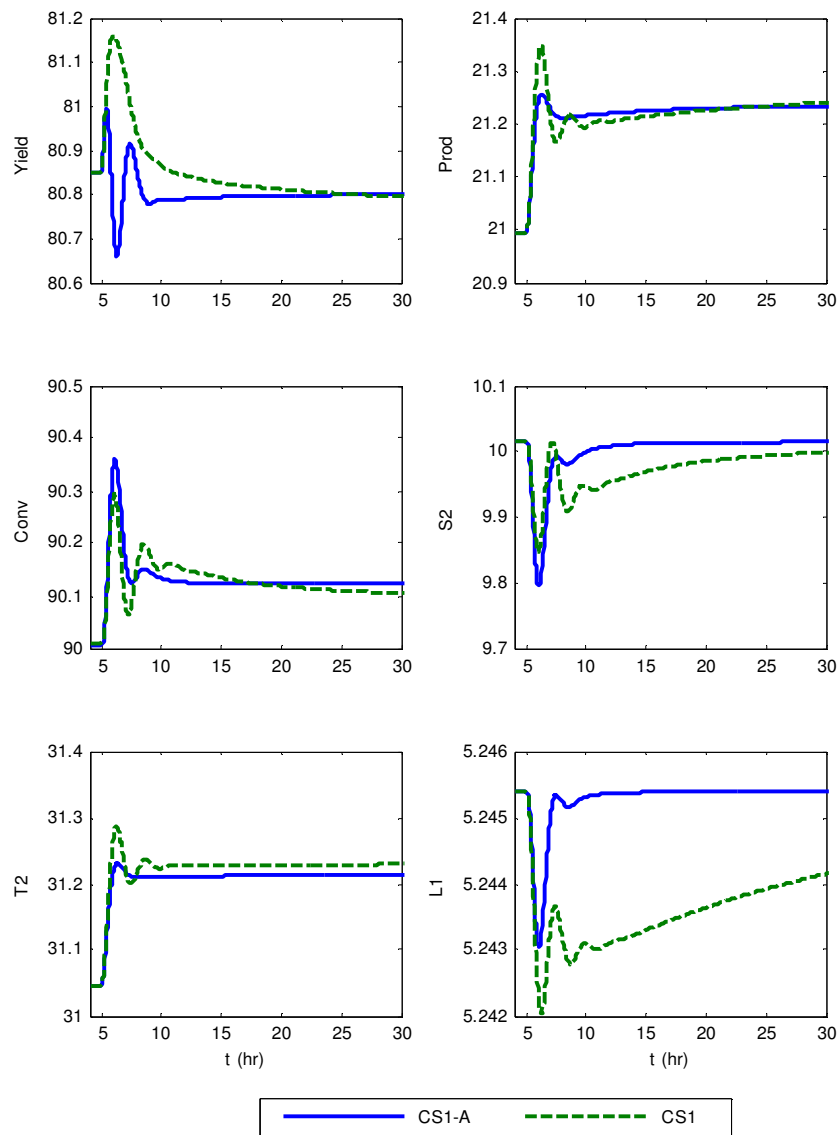


Figure 8-17: Dynamic responses of performance measures and controlled variables correspond to step change in fresh stream temperature, $\Delta T_o = 1.0^\circ\text{C}$

8.5.3 Implication of Different Control Strategies on Variables Interaction

Note that from the previous Chapter 7, the implementation of the CS1 has changed the nature of variables interaction – closed-loop variable interaction is different from that of the open-loop for case of large variations in S_o (magnitude of change equals to 30kg/m^3). It can be seen from Figure 8-13 that under the CS1, the responses of inventory and constraint variables i.e. pairs $(L_1 \text{ and } L_2)$ and $(T_1 \text{ and } T_2)$ are opposite to each other, hence implies they are negatively correlated under the closed-loop system. However, from the previous PCA-based analysis (open-loop system), we discovered that the pairs $(L_1 \text{ and } L_2)$ and $(T_1 \text{ and } T_2)$ are positively correlated with each other. Hence, this means that the variables interactions under the open-loop and closed-loop systems are different. *The question is, to what extent does this difference affects the performance of a given partial control strategy?*

To answer this question it is important to bear in mind that, the central objective of PCA-based partial control design is to harness the benefit of variables interaction in such a way that the *external* control system functions synergistically with the *inherent control system* of a given process. Here, the inherent control system means that the natural tendency of the open-loop process to regulate itself e.g. self-regulating system. The existence of such an inherent control system is prevalence in most of the biological systems where the living microorganisms have the capacity to regulate their own environments. Meanwhile, the term external control system is referring to our choice of control strategy to control a given process. It is imperative for an effective control system design that both external and inherent control systems must work cooperatively in order to achieve a given set of operating objectives. And the key to achieving this important goal is to understand the process variables interaction.

Understanding of the variables interaction is essential because it ultimately determines two important decisions governing an effective design of control strategy:

- 1) Which variables should be controlled (selection from the candidates)?
- 2) How many variables should be controlled?

These two decisions can be made following the PCA-based analysis which is actually an open-loop analysis. Accordingly, it is important to remember that, the result of the variables interaction analysis determining the two decisions above is from the

open-loop viewpoint. It follows that the main assumption of the partial control design based on this analysis is that, the resulting (external) control strategy design must preserve the open-loop variables interaction. Consequently, if the variables interaction is altered by the implementation of a chosen control strategy, we then expect that the performance of this control strategy will be *sub-optimal*. In other words, sub-optimal performance implies the deviation of the actual performance (e.g. variations in performance measures and dynamic responses) from what can be predicted from the result of open-loop PCA-based analysis. It should be remembered that such a sub-optimal performance is the result of the non-cooperative nature of the chosen control strategy with the inherent control system of a given process.

Now it becomes clear apart from the presence of BCL, the reason why the performance of CS1 is inferior to CS1-A and CS1-B (especially with large magnitude of disturbance) is due to the non-cooperative nature of CS1 with the inherent control system – design which does not lead to the synergistic external-inherent control system. When the disturbance magnitude is small (only 10kg/m^3), the inventory variables under the CS1 (Figure 8-15) seem to regain their positive correlation (although their extent of interaction has now been weakened), and hence the SEIC property is improved. As a result, the performance of CS1 in this case is almost comparable with that of the CS1-A. In conclusion the better the SEIC property, the better is the expected performance of the control system involved.

For a large disturbance magnitude, evidence of this non-cooperative nature is given by the fact that the closed-loop variables interaction (under the CS1) is different from that of the open-loop. On the other hand, the 3x3 control strategies (CS1-A and CS1-B) yield improved performance not only because of the BCL elimination from the control systems but also due to the preservation (minimization of the change) of the open-loop variables interaction. In other words, the 3x3 control strategies work synergistically with the inherent control system of the process; this is shown by the preservation of the open-loop variables interaction.

Now we can summarize that the bottom-line for an effective partial control design requires the fulfillment of two most *critical* conditions:

- 1) Elimination of BCL from the control system.

- 2) Preservation of the open-loop variables interaction by the implementation of a chosen control strategy.

Meeting these two conditions requires that the partial control strategy must be of certain size which is neither too large nor too small i.e. must be of optimal size. While the large size (too many controlled variables) can lead to the presence of BCL and possible alteration of the open-loop variables interaction, a size which is too small can lead to unacceptable variations in the performance measures. Dealing with this dilemma requires an effective tool to determine the sufficient number of controlled variables, such as the dominant variable interaction index (I_{DV}) proposed in this thesis.

8.5.4 Summary of Performances Comparison for CS1, CS1-A and CS-B

Table 8-1 shows the integral absolute error (IAE) for CS1, CS1-A and CS-B for the case of $\Delta S_o = 30\text{kg/m}^3$. Obviously, the IAE values for CS1-A and CS-B are much smaller than that for CS1. The most drastic improvement with the implementation of CS1-A and CS1-B is on the reduction of IAE for the *Prod* – much faster recovery of *Prod* under these two strategies than under CS1. Note that, even without PID enhancement the performance of CS1-A is much better than that of CS1 which is augmented with feedforward control. Of course, with the feedforward control enhancement the CS1-B shows quite a significant improvement over CS1-A especially in term of reduced IAE value for the *Conv*. From steady-state point of view, however, both CS-A and CS-B show almost equal improvement in performance over the CS1 in term of the variation in *Yield*.

Table 8-2 shows the dynamic performance (in term of peak change during transient response) of the inventory-constraint variables. The CS1-A and CS-B show large improvement over CS1 in terms of reduced peak values in T_2 , L_1 and L_2 . Unlike in the case of IAE for performance measures, both CS1-A and CS1-B exhibit comparable performance. In summary, with the optimal size of partial control strategy, we can afford not to use any PID enhancement technique. Therefore, the right size of control systems is fundamental in achieving the control objectives.

Table 8-1: Performance measures under different control strategies: $\Delta S_0 = \pm 30 \text{ kg/m}^3$

Performance Measure, Φ	Yield (%)			Conv (%)			Prod ($\text{kg/m}^3\cdot\text{hr}$)		
	CS1	CS1-A	CS1-B	CS1	CS1-A	CS1-B	CS1	CS1-A	CS1-B
IAE ₁₀₀	27.41	15.07	11.21	29.26	9.68	4.44	10.34	1.4	0.81
$\Delta\phi$ (%)	0.03	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01	< 0.01

IAE₁₀₀ - integral absolute error taken up to 100 hours in simulation time**Table 8-2: Maximum peak change ($\Delta y_{\max, \text{dyn}}$) of variables under different control strategies: $\Delta S_0 = \pm 30 \text{ kg/m}^3$**

Variable, y	T ₂ (°C)	T ₁ (°C)	Et ₂ (kg/m^3)	L ₁ (m)	L ₂ (m)
CS1	32.1	30.7	41.9	5.34	6.65
CS1-A	31.1	30.1	41.6	5.28	4.22
CS1-B	31.2	30.1	41.2	5.33	4.22
Nominal value	31.0	29.9	41.2	5.24	4.20

8.6 Summary

For an effective partial control design, two important conditions must be fulfilled:

1. Elimination of BCL from the control system design.
2. Preservation (or minimization of change) of the open-loop variables interaction by the implemented control strategy.

The bottleneck control loop (BCL) is defined as the control-loop which is responsible for limiting the dynamic performance of a given control system. It is crucial to remove the BCL rather than attempting to alter the controllers tuning in order to increase the speed of the overall dynamic responses. To eliminate the BCL from the control system, we can employ the SVD analysis in order to detect the presence of BCL. If the minimum singular value of KP ($\underline{\sigma}(KP) \ll 1$) is very small less than unity, then this indicates the presence of BCL in the control system. Here K and P are the control system and linearized plant model respectively. For a good control system (with no BCL), it is desirable that $\underline{\sigma}(KP) \gg 1$. In the case study, the F_1-rx_2 has been identified as the BCL (in the preliminary analysis) which is confirmed by the SVD analysis.

Meeting the second condition is the central goal in the effective partial control design, which is to ensure that the chosen (external) control system can work synergistically with the inherent control system of a given process. This goal can be achieved if the nature of open-loop and closed-loop variables interaction is similar. It is important to note that, this is also necessary because the PCA-based analysis is an open-loop analysis. Therefore, the second condition arises from the main assumption that the open-loop variables interaction must be preserved by the control system implemented.

From the partial control design perspective, the elimination of BCL and preservation of open-loop variable interaction requires a certain size of control strategy. A size which is too large (too many controlled variables) tends to introduce BCL and alter the open-loop variables interaction, which in turn lead to sub-optimal performance of the control strategy. On the other hand, the size which is too small (very few controlled variables) can lead to the unacceptable variations in performance measures and perhaps leads to lack of robustness against disturbances. Thus, there must be a trade-

off size which can be determined using a tool such as the dominant variable interaction index i.e. to determine the sufficient number of primary controlled variables.

The simulation results of three different control strategies show that the 3x3 control strategies (BCL i.e. F_{I-rx_2} is removed) displays superior performance to the 4x4 control strategy. Even without the feedforward enhancement, the 3x3 control strategy (CS1-A) exhibits significantly better performance than the 4x4 control strategy which is augmented with the feedforward control, in terms of:

1. Faster settling time of variables (controlled and uncontrolled) and the performance measures.
2. Lower peak changes during the transient period of inventory-constraint variables and performance measures (i.e. smaller IAE values for *Yield*, *Conv* and *Prod*).

Lower fluctuations (or peak changes) of the inventory variables under the 3x3 control strategies means that we can push the operation of bioreactor closer to its maximum volume, which in turn can generally lead to economic benefit. Interestingly, the implementation of the 3x3 control strategy does not lead to a significant loss in the steady-state performance - the variations in the performance measures remain acceptable. This is expected from the result of analysis using the so-called dominant variable interaction index (I_{DV}).

It is important to point out that the implementation of the 3x3 control strategy does not change in a very significant way the open-loop variables interaction – both open-loop and closed-loop variables interaction is more or less similar. In this case, for example, both L_1 and L_2 show positive correlation (similar to the open-loop correlation) under the 3x3 control strategies. In addition, the implementation of the feedforward control (CS1-B) apparently does not change the open-loop variables interaction.

An important conclusion that can be drawn from this case study is that, a large number of controlled variables even if we can afford it (i.e. large number of manipulated variables is available) will not necessarily lead to a better performance than that of a small number of controlled variables. Indeed in partial control approach, the size of controlled variables set is extremely important in determining the effectiveness of the resulting control strategy; the study suggests that the smaller control system does not mean inferior to larger and more complex control systems.

9 CONCLUSIONS AND RECOMMENDATIONS

9.1 Conclusions

Almost four decades have passed since the critique of chemical process control theory by Foss in 1970s (1973) in which, he highlighted the gaps between the theory and practice in process control. His critique has ever since provided motivation and guidance to researchers in one of the most important design problems in modern process control today, known as the control structure design (CSD). The reason why CSD is very important is because it relates to the *control philosophy* of overall plant and as such, demands answers to 3 important questions: which variables to be controlled, which variables to be manipulated and what is the structure interconnecting these two sets of variables? Although it has long been realized that the impact of control structure design is far more important than the controller algorithm design, it is the latter which has enjoyed large research attentions in process control community. Perhaps this is not surprising because CSD is a very difficult, open-ended problem for which there is no precise mathematical formulation - hence it has no unique solution.

Nevertheless research study in the last 3 decades into control structure problem has led to the development of various methods that can broadly be categorized into two major families: (1) mathematical approach, and (2) heuristic-hierarchical approach. Both approaches have their own advantages and limitations.

9.1.1 Advantages and Limitations of Current CSD Approaches

The primary advantage of mathematical approach such as the self-optimizing control structure method lies in its solid theoretical foundation within which the control structure problem can be addressed in a systematic manner. Moreover, such a theoretical foundation allows engineers to translate the set of control objectives which could be *implicit in nature* into a set of controlled variables. In fact, this is the fundamental issue to be resolved within CSD problem. Despite its attractiveness from theoretical

perspective, mathematical approach suffers from several limitations which probably have prevented its widespread acceptance in process industries. One of the main limitations is its reliance on mathematical optimization, which becomes impractical for systems with large number of input-output variables. When the number of input-output variables is large then this leads to prohibitively large number of control structure alternatives, which in turn leads to enormous computational effort. The second important limitation arises from the nonlinearity of the process system, which frequently leads to non-convex optimization. As a result, the solution of mathematical-based method might be sub-optimal. And the third important limitation associated with the mathematical approach is the difficulty in formulating the optimization problem, especially when it comes to multiple control objectives formulation. In this case, one of the main challenges is how to specify the weight on each of the control objectives.

On the contrary to mathematical approach, the heuristic-hierarchical approach, for examples, the 5-tiered framework and 9-step procedure has enjoyed better acceptance among the industrial practitioners due to its simplicity. It is interesting to note that, many of the methods within this category still inherit the *characteristics* of dynamic process control concept, which was introduced by Buckley (1964) in 1960s. Notwithstanding its simplicity from the practitioners' point of view, the heuristic-hierarchical approach possesses some limitations inhibiting its effective applications in process industries. One of these limitations arises from its heavy reliance on process knowledge and engineering experience. As such, the implementation of this method may not work well on a new process (or unfamiliar process) where experience about the process is scarce. Additionally, the novices will find it hard to implement this approach even to a familiar process because of their lack of experience. Even more serious limitation of heuristic-hierarchical approach arises from its lack of theoretical foundation. As a result, it is not convenient (or even possible) to translate the set of control objectives especially those which are implicit in nature, into a set of controlled variables in a systematic manner. Hence, this frequently leads to the adoption of *ad-hoc* procedures in the selection of controlled variables in particular.

9.1.2 Data-Oriented Approach to Solving CSD Problem

9.1.2.1 Theory

In this thesis, we propose a novel data-oriented approach to solving control structure problem with an emphasis on the controlled variables selection. It is interesting to note that, the proposed approach represents a significant departure from the existing mainstream approaches in CSD. The approach is essentially the result of the integration of two major concepts, which are known as partial control structure (PCS) and principal component analysis (PCA).

The PCS approach has been widely applied in process industries since the beginning of modern process control era because it can lead to simple and cost-effective control systems. Surprisingly, despite decades of industrial practice there has been no systematic tool or procedure available for the effective implementation of partial control strategy. In the absence of systematic tool, in most cases the implementations are done in a rather ad-hoc manner relying heavily on process engineering experience. As such, partial control also suffers from similar limitations as that of heuristic-hierarchical methods. But unlike heuristic-hierarchical methods, the PCS is built on a sound theoretical foundation, which has the potential to guide the engineers in selecting the controlled variables, known as the *dominant variables*. However, it is doubtful that the current practice relying heavily on engineering experience is able to realize this advantage – systematic tool is required.

In view of the shortcomings of existing partial control framework, which relies heavily on process experience, we propose in this thesis a modification of this framework in such a way to accommodate the application of a novel PCA-based technique for identifying the so-called dominant variables. Whereas in the generalized (classical) concept of partial control, the control objectives are implicitly lumped together into a set of variables known as the *performance variables*, in the refined (new) concept of partial control framework the control objectives are strictly divided into 3 main categories: (1) overall (implicit) performance objectives or measures, (2) constraint control objectives, and (3) inventory control objectives.

Accordingly, the distinguishing feature between the classical and new frameworks rests on the significance of dominant variables. In the classical framework the significance of dominant variables is attached to all 3 types of control objectives i.e. overall, constraint and inventory control objectives. We believe this approach is at most only capable of meeting the constraint and inventory control objectives and not the overall performance objectives. The reason is that, it is not convenient (i.e. far from obvious) or even possible to translate the implicit performance measures into a set of controlled variables based on experience without any systematic tool. As a consequence, the classical framework is likely to lead to *sub-optimal* control strategy that can only achieve the inventory and constraint control objectives.

Conversely, within the new framework we attach the existence of dominant variables only to the overall performance measures, which are normally implicit functions of process variables. Therefore, it follows that the search for the dominant variables is restricted only to finding, which variables that are strongly linked to the overall performance measures. Also note that, within the new framework of PCS this task is accomplished through a systematic tool known as the PCA-based technique. Unlike the dominant variables relating to the implicit performance objectives, the variables which define the inventory and constraint control objectives can normally be identified directly from process (unit operation) knowledge, and thus, no specific tool may be required to identify them i.e. no substitute to good knowledge.

Within the new theoretical framework of partial control, not only that a tool (PCA-based technique) is introduced to identify the dominant variables but also a clear definition for the dominant variables is established. Bear in mind that, there has been no proper definition for the dominant variables within the context of generalized framework of partial control. It is important to note that, the keys to successful application of this PCA-based technique are the fulfillment of 3 important factors: (1) dominant variable (DV) criteria, (2) successive dataset reduction (SDR) condition, and (3) critical dominant variable (CDV) condition.

Having identified the set of dominant variables, an important question then follows; do we need to control all of the dominant variables, which in this thesis are referred to as the *primary control variables*. Also the same question can be asked for the case of

inventory and constraint variables once we have fully identified them via unit operation knowledge. Surprisingly, the key to answering this question hinges on our understanding of the so-called *variables interaction*.

When the candidate (dominant or inventory or constraint) variables are strongly interacted or correlated among each other, then it is not necessary to control all of them. Therefore, even if we only control a subset of the candidate variables, the other variables will be indirectly controlled by virtue of their interaction with the controlled variables. Then, this leads further to other important questions: (1) which candidate variable/s should be controlled, and (2) how many variables should be controlled? With regard to the first question, the answer depends on the type of control objectives.

For the overall control objectives, we introduce the concept of closeness index (CI) to rank the influence of each dominant variable on the performance measure/s. Of course, the most influential dominant variable should be controlled. As for the inventory-constraint variables, we can rank the significance of each variable based on process knowledge e.g. the constraint variable that is known to be the most critical must be controlled. To augment the ranking analysis, we also propose heuristic guidelines to select the primary, inventory and constraint controlled variables from their corresponding candidate variables.

Next, to answer the second question we propose two quantitative tools known as: (1) dominant variable interaction index (I_{DV}), and (2) variable-variable interaction index (I_{VV}). Both indices are derived from the concept of closeness index. The I_{DV} is used to assess the sufficient number of dominant variables that needs to be controlled, which will lead to acceptable variations in performance measures. Likewise, I_{VV} is used to assess the sufficient number of inventory-constraint variables to be controlled such that, the variation of the other uncontrolled inventory-constraint variables are within an acceptable range in the face of external disturbance occurrence.

9.1.2.2 Application and New Insights

The data-based approach of partial control incorporating the PCA-based technique is successfully applied to the case study: the two-stage continuous extractive (TSCE) alcoholic fermentation system. This system exhibits strong nonlinear behaviour arising

from the complex kinetics of the yeast used – dynamic controllability analysis (Chapter 5) indicates that the strong nonlinear behaviour can pose difficulty to control system design. Some new insights crystallize from the nonlinear simulation study as follows:

1. It is possible to design a basic partial control strategy for the TSCE alcoholic fermentation system, which focuses only on the performance measures – this will normally lead to the smallest size partial control system. However, it should be remembered that whether the basic partial control strategy is able or not to stabilize a system, and at the same time ensures acceptable loss in performance measures due to disturbance occurrence depend very much on the system of interest.
2. It is shown that the set of dominant variables is non-unique from the classical partial control framework viewpoint because of the variables interaction.
3. Variables interaction is the working principle governing the partial control strategy – thus, understanding this interaction is crucial for an effective partial control design.
4. The effectiveness of partial control strategy depends on two critical conditions:
 - a) The presence of bottleneck control loop (BCL), which imposes limitation on overall control system performance must be avoided. Singular value decomposition (SVD) analysis on KP can be used to detect the presence of BCL in the control system K which is applied to a plant P .
 - b) The open-loop variables interaction must be preserved by the implementation of the (external) partial control strategy. When this condition is fulfilled then, we say that the *external* control strategy works synergistically with the *inherent* control system of a given process.

In 1970s Foss raised 3 important questions which finely articulated the essence of control structure problem: *which variables to be controlled, which variables to be manipulated and how these two sets are connected?* But in light of the study described in this thesis, there is a reasonable ground to believe that these are not the only *philosophical questions* we should seek to answer when dealing with CSD problem. Just as important question requiring careful consideration is *how many variables should be*

controlled? Unfortunately, this last question has never been raised before in the history of CSD research.

The last question points to the significance of variables interaction which is recognized in this thesis as the working principle governing the partial control design. In other words, we cannot design an effective partial control strategy without proper understanding of the nature of variables interaction possessed by a particular process of interest. It is important to note that, unless we address the last question in a systematic manner, there is a great possibility that the resulting control system will be *non-optimal* in size i.e. either too many or too few controlled variables.

Finally, though research work in control structure problem has spanned over 3 decades, the bulk majority of methods developed over this time period has ignored the significance of variables interaction. As process systems are characterized by variables interaction, it is hard to believe that the current mainstream methods for solving the CSD problem are capable of producing an optimal size control system. In this regard, the proposed data-based approach (or more specifically PCA-based technique) described in this thesis represents the first method, which can systematically deal with the process variables interaction – thus, makes it possible to determine the optimal size of control system.

9.1.3 Key Advantages of Data-Oriented Approach

The dynamic simulation results in this work demonstrate that the proposed data-oriented approach has the capability of unifying the advantages of both mathematical and heuristic-hierarchical approaches. Even more interesting, it can effectively overcome the limitations faced by these two mainstream approaches. In short, we can identify the advantages of the data-oriented approach as follows:

1. It shares the primary advantage of mathematical approach in the sense that it has a sound theoretical foundation, which is based on the concept of partial control. Hence, it enables the engineers to address the CSD problem in a systematic manner.
2. Unlike mathematical-approach, the data-oriented approach does not require any optimization. Also it can be applied to real plant as well as to simulated plant.

Note that, it is not possible to directly applied mathematical-approach to real plant.

3. It is simple to follow and yet it provides effective solution to the complex CSD problem in the sense that, the resulting control system is simple, i.e. low dimension.
4. The PCA-based technique makes it possible for the engineers to identify the dominant variables without the need for rigorous process engineering experience.
5. Within the refined framework of partial control, the PCA-based technique can help the engineers to gain insights into the nature of variables interaction (i.e. output-output variables interaction). Neither mathematical nor heuristic-hierarchical approach is capable of handling this variables interaction in a systematic manner.

9.2 Recommendations

We suggest the following for further improvement and future research direction for the data-oriented approach:

1) *Robustness*

If the approach is applied to real plant, then one of the important issues is the robustness of the analysis using the proposed PCA-based technique against noise in the measurement data. Filtering technique to remove the effect of noise from the measurement data is required, such that the PCA-based technique can reliably be applied.

2) *Extension of the approach to multi-scale system*

Currently the approach is applied to a system which is modeled based on the *unstructured* (macroscopic) *kinetics* – hence, it is a single-scale system. Bioprocess can be modeled based on the structured metabolic model which will lead to multi-scale system. In near future it will become possible to control both macro- and micro-scale variables leading to multi-scale control system. So, extension of the current approach to multi-scale system can facilitate the *multi-scale control structure design* in biotechnological processes.

3) *Extension to decentralized model predictive control (MPC) design*

Decentralized MPC design for large-scale system is a challenging issue where, the best approach is probably based on the *corporation* scheme. In this scheme the algorithm is developed in such a way that the interaction among the MPCs is directly taken into account. But this scheme requires more complex and heavy computational effort than the completely *decentralized* MPC scheme. Thus, we ask ourselves a question, is it possible to design a decentralized MPC system without modifying the original algorithm as in the case of complete decentralized scheme? A lesson from the partial control study in this thesis points to the importance of understanding variables interaction. From this perspective, the system can be decomposed using the PCA-based technique (perhaps modification of its existing form is required) to yield groups of candidate variables. Note that, the variables interaction must be strong within each group but must be negligible across different groups. Then, a separate MPC is designed to control selected variables for each group – this is to ensure minimum interaction among the MPCs. It is important to note that, however, this approach is in a sense resembles that of partial control using completely decentralized PID controllers. The only difference is that the number of controllers is reduced for the case of decentralized MPC. We think this might lead to a better result than the currently complete decentralized (or even corporation) MPC scheme, although we let the future study speaks for the validity of this presumption.

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