PLANT-WIDE CONTROL OF INDUSTRIAL PROCESSES USING RIGOROUS SIMULATION AND HEURISTICS

N.V.S.N. MURTHY KONDA

NATIONAL UNIVERSITY OF SINGAPORE

2006

PLANT-WIDE CONTROL OF INDUSTRIAL PROCESSES USING RIGOROUS SIMULATION AND HEURISTICS

N.V.S.N. MURTHY KONDA

(B.Tech., National Institute of Technology, Warangal, India)

A THESIS SUBMITTED

FOR THE DEGREE OF DOCTOR OF PHILOSOPHY

DEPARTMENT OF CHEMICAL AND BIOMOLECULAR ENGINEERING

NATIONAL UNIVERSITY OF SINGAPORE

2006

To My Family

&

Foster Parents

ACKNOWLEDGEMENTS

I consider myself blessed to be a doctoral student of Prof. Rangaiah. I would like to express my deepest gratitude to him for his continuous support, invaluable suggestions and constructive criticism, which enhanced my independent and critical-thinking and buttressed my thesis. Under his guidance, I have learnt two important questions that a researcher should always ask him/her-self: *Why* and *How*. I believe that these two elements are essential for a productive research, and would enable me to carry out the same in future. In addition, he has been very kind and caring; and thanks for all his encouragement especially during untoward conditions. I will always cherish the moments that I spent with him during Deewali gatherings and long-drive to Malaysia.

I would also like to express my gratefulness to my co-supervisor, A/Prof. Krishnaswamy, for sharing his practical-insights and scientific-knowledge. I am thankful to Prof. Raj Rajagopalan, Dr. Tong, Dr. Yung and A/Prof. Raj Srinivasan, who always encouraged us, despite their busy schedule, to take part in the activities of GSA. I am grateful to Dr. Laksh, for being a constant source of inspiration to me. The stimulating technical and non-technical discussions that I have had with Dr. Laksh and his group members are very thought-provoking and informative. My cordial acknowledgements to A/Prof. Chiu (for teaching me the basics of multivariable control), Prof. Karimi and A/Prof. M. P. Srinivasan, from whom I learnt design principles and complex distillation synthesis, respectively, during tutorials. I am also thankful to Mr. Boey, Mrs. Khoh and Ms. Fam for helping me on several lab and equipment related issues.

I am indebted to Ganesh and Mranal, the kingpins amongst all my friends, without whom I would not have come to NUS. I am fortunate to have sincerest lab-mates like Srinu, Rampa, Naveen, Abhijit and Suraj, and naughtiest flat-mates like Anan, Sendhil, Vipul and Tanu. I am sincerely thankful to Chandra, Prabhat and Madhu for enlightening my technical fundamentals. I am immensely thankful to my career-advisors Pavan, Ravindra Marathe and Suresh. Thanks to my tennis-mates (Suresh, Ganesh and Ramki) and tennis-guru (Mranal) for their jovial companionship; I wonder whether I would ever be able to beat them in tennis. My heartiest thanks to Sunil, Dada, Ravi, Gaurav, Santanu and Khalid without whom, I would not have gotten so familiarized with the scenery of Malaysia. Raaj and Sirisha, the nicest couple I have ever seen, deserve special gratitude; the moments that I spent at their place reminded me of my home. Special thanks to Lalitha, Arul, Mohan, Biswajit, Manish, Ayman, Karl, Naveen, Avinash, Ankush, Sudhakar, Reddy, Sreenivas, Satish, Raghu, Balaji, Suresh, Mukta, Amrita, Karthiga, Vivek and Sundar, who made my journey through GSA activities more enjoyable. In addition, I will always be indebted to my bachelors' cronies Ajay, Kris, Bajian and LND, who have gone out of their ways to help me, and Kittu, for teaching me the basics of Chess.

I would like to express my endless gratitude to my parents, foster parents, the human dynamos – my brother and sister for their everlasting love which, emphatically, helped me to become what I am now. Last but not the least, I would like to extend my gratitude to National University of Singapore for providing the opportunity for, and financially supporting my doctoral studies.

TABLE OF CONTENTS

SUMMARY

Due to the globalization of chemical process industry in the late 20th century, the need for efficient and effective processes is now more than ever. In order to stand out in the competitive marketplace, every industry is becoming increasingly aware of the fact that the processes have to be more economically attractive, environmentally benign and customer-centric. Hence, one of the primary challenges of the process systems engineer in the modern world is to investigate and implement the methods to design sustainable processes and control systems to achieve the best possible returns. In order to improve the economic feasibility, processes need to be tightly integrated (with material and energy recycles) which would typically complicate the analysis and pose unforeseen safety and operational difficulties. In addition, constantly changing market demands, ever-tightening environmental policies and safety regulations make it even more difficult to control and operate the plant. Given this scenario, how does a present-day engineer address it? Do we have systematic and reliable methods and tools to make use of? The present work is aimed at providing effective solutions to these issues.

First, a comprehensive review of various plant-wide control (PWC) methodologies in the literature is carried out, and a systematic classification of PWC methodology is presented. Then, a methodically-driven integrated framework, that capitalizes the strengths of both the heuristics and rigorous simulation tools, is proposed. The basic idea here is to decompose the complex task of PWC system design into a number of relatively simple steps, and to make use of both the simulation tools and heuristics at every stage to arrive at the final solution. The main function of the rigorous nonlinear simulation is to improve the accuracy of decision by reducing the over-reliance on heuristics and to improve the process insight through

virtual hands-on experience; while the main function of heuristics is to simplify the analysis of the seemingly complex task by quickly screening the alternatives. Secondly, a simple and effective procedure for control degrees of freedom is proposed and then successfully applied to highly integrated processes.

Thirdly, a new metric called ‘Dynamic Disturbance Sensitivity (DDS)’ is proposed to gauge the dynamic performance of alternate control structures and process designs using rigorous nonlinear dynamic simulation. The idea is to use the inherent correlation between process dynamic performance and component accumulation as a measure. More specifically, DDS is defined as the sum of absolute accumulation of all the components and is successfully used to show the superiority of the proposed PWC method by comparing the dynamic performance of the resulting control systems with that of existing ones in the literature.

Finally, the feasibility of a recent and improved process design procedure is critically analyzed. A modified sequential approach is then proposed by combining the proposed PWC methodology with the improved process design methodology to study the interaction between design and control from plant-wide perspective. It is successfully applied to generate and evaluate several process designs and their control systems for HDA process.

The studies and findings outlined above should facilitate realistic PWC system design as well as increased use of rigorous dynamic simulations in both the academia and industry.

NOMENCLATURE

Abbreviation	Explanation
AI	: Artificial Intelligence
CC	: Composition Controller
CCD	: Control Configuration Design
CDOF	: Control Degrees of Freedom
CLDG	: Closed Loop Disturbance Gain
CN	: Condition Number
COSMO	: Conductor-like Screening Models
CSTR	: Continuous Stirred Tank Reactor
CV	: Controlled Variable
DAE	: Differential Algebraic Equations
DCN	: Disturbance Condition Number
DDS	: Dynamic Disturbance Sensitivity
DOF	: Degrees of Freedom
DMC	: Dynamic Matrix Control
EG	: Ethylene Glycol
EO	: Ethylene Oxide
FC	: Flow Controller
FEHE	: Feed-Effluent Heat Exchanger
HDA	: Hydrodealkylation
IDA	: Input Disturbance Alignment
IDGD	: Input-Disturbance Gain Deviation
ILP	: Integer Linear Programming
IMC	: Internal Model Control
IMCIM	: Internal Model Control Interaction Measure

LC	: Level Controller
mAHP	: modified Analytical Hierarchical Process
MILP	: Mixed Integer Linear Programming
MIMO	: Multi Input Multi Output
MINLP	: Mixed Integer Nonlinear Programming
MPC	: Model Predictive Control
MV	: Manipulated Variable
MVC	: Minimum Variance Control
NI	: Niederlinski Index
NMPC	: Nonlinear Model Predictive Control
NRTL	: Non-Random-Two-Liquid
OP	: Controller Output
PC	: Pressure Controller
PDAE	: Partial Differential Algebraic Equations
P-F	: Pressure-Flow
PFR	: Plug Flow Reactor
PG	: Propylene Glycol
PID	: Proportional-Integral-Derivative
PO	: Propylene Oxide
PR	: Peng-Robinson
PRG	: Performance Relative Gain
PV	: Process Variable
PWC	: Plant-Wide Control
RDG	: Relative Disturbance Gain
RGA	: Relative Gain Array
RSR	: Reactor-Separator-Recycle
SDS	: Steady-State Disturbance Sensitivity
SEA	: Snowball Effect Analysis

SIE	: Single-Input Effectiveness
SISO	: Single Input Single Output
SP	: Set Point
SVA	: Singular Value Analysis
SVD	: Singular Value Decomposition
TC	: Temperature Controller
TE	: Tennessee Eastman
TPM	: Throughput Manipulator
VCM	: Vinyl Chloride Monomer
VLE	: Vapor-Liquid Equilibrium
WCIDG	: Worst Case Input-Disturbance Gain

Symbols	**Explanation**
CH_4	Methane
d_k	k^{th} disturbance
H_2	Hydrogen

Subscripts	**Explanation**
R	Recycle
R-in	Reactor Inlet
in	Inlet
out	Outlet

LIST OF FIGURES

LIST OF TABLES

CHAPTER 1

INTRODUCTION

1.1 Plant-Wide Control (PWC)

In order to keep pace with the growing global competition and customer demands, chemical processes need to deliver products with consistent quality but at lower cost. Besides, due to the stringent environmental regulations and safety measures, healthier processes that are more environmentally-benign and operator-friendly are required. More often than not, all these aforementioned objectives call for effective and efficient control systems. On the other hand, cost-effective process design usually results in a complex and highly integrated process with material/energy recycles; safety issues then become more prevalent and maintaining consistent product quality also becomes more difficult. Likewise, inventory levels tend to be kept low, especially when expensive/dangerous chemicals are involved, to improve plant-economics and safety; but this introduces several adverse effects on plant operation (Luyben and Hendershot, 2004). From this discussion, it follows that one of the challenges of a process systems engineer is to design effective control systems for complex processes (Keller and Bryan, 2000), which necessitates the development of systematic procedures to synthesize more efficient control systems.

Plant-wide control (PWC) in general refers to designing efficient control systems for highly integrated processes to satisfactorily achieve demands on production rate and product quality without violating environmental and safety regulations. Due to the presence of large number of unit operations and control loops, PWC is also referred to, though less common, as ‘large scale system control’ (e.g., Turkay et al. 1993; Doyle et al., 1997; Vadigepalli and Doyle, 2003) and 'network control' (e.g., Baldea et al., 2006) in the literature. Similar to process design, which can be done using several techniques such as evolutionary synthesis and superstructure optimization (Johns, 2001), PWC systems can also be designed by different methods. Chapter 2 discusses several of these methods. Whatsoever the PWC methodology, by and large, the basic control system design procedure remains the same and involves three main steps (Skogestad and Postlethwaite, 1996):

1. Control Structure Design (Structural decisions)
2. Controller Design (Parametric decisions)
3. Implementation

Control Structure Design can be subdivided into the following steps (Skogestad and Postlethwaite, 1996; Stephanopoulos and Ng, 2000).

1. Identification of control objectives.
2. Selection of controlled outputs with set points.
3. Selection of manipulated inputs (which include not only control valves or flowrates to manipulate, but also flow ratios, sums or differences of flow rates, heat removal or addition rates etc.)
4. Selection of measurements for control purposes.
5. Selection of control configuration/controller structure (i.e., how to pair the controlled and manipulated variables in case of decentralized multi-loop single-input single-output, SISO control system)
6. Selection of controller type (e.g., proportional-integral-derivative, PID controller)

For a simple distillation column, there can theoretically be more than 120 control configurations. When it comes to an entire plant, what makes PWC system design even more complex is the possibility of multitude of alternative control structures. For instance, for a medium-scale industrial process such as the

Tennessee Eastman (TE) process, 4×10^7 alternative control structures are possible (Kookos and Perkins, 2001a). The problem is compounded by another challenging feature of industrial processes with recycles - the cyclical propagation of the effect of disturbances between upstream and downstream operations irrespective of where the disturbance(s) originated. To complicate the matter further, recycles often introduce other problems spanning from increased interactions among process variables to increased nonlinearity (Bildea and Dimian, 2000; Kumar and Daoutidis, 2002). In addition, at times, recycles can even lead to process instability. In short, the problems due to recycles not only make the PWC system design complex but also demand good co-ordination of control actions among various sections of the plant. Hence, any PWC system should take these into account and be able to nullify the ill-effects of recycles as much as possible to improve the overall performance.

1.2 Motivation and Scope of the Work

It is evident from the above discussion that the contemporary chemical processes are becoming increasingly complex mainly due to the presence of recycles. Thus, this research is primarily fuelled by the increasing process complexity and the need for practical PWC system design methods. The work on this front has been relatively sparse prior to 1990s mainly due to the unavailability of powerful tools/techniques. However, there has been growing attention from the researchers in this direction over the last 15 years. In this thesis, we try to shed more light on the issues which have either received less attention or solved partially. For example, rigorous process simulation models, despite their usefulness in PWC studies, have not been used extensively in the past. So, one of the objectives of the present thesis is to effectively use rigorous simulation models (steady-state and dynamic) in order to extract more accurate information which in turn leads to better decisions. Such simulation tools are observed to be indispensable for plant-wide studies as it is extremely difficult, expensive and tedious to carry-out plant-wide experiments.

Due to increasing process complexity, not only PWC system design but process design also becomes more difficult. Hence, we have also examined the applicability of the conventional design procedures to the modern chemical processes and studied the interaction between design and control from the plant-wide perspective. In addition, the thesis encompasses other relevant issues such as performance assessment of PWC systems. All these aspects, along with brief motivation, are discussed below.

Classification of PWC Methods: There have been several approaches to PWC system design but very limited attention is paid towards systematically classifying these PWC approaches; such a classification would indeed give a quick overview of these methods to researchers in the PWC community. Hence, these methods are systematically classified and the uses of such classification are discussed in the Chapter 2.

Integrated Framework for PWC: Luyben et al. (1999) have proposed a 9-step heuristic procedure to design PWC systems which is lately cited in textbooks (e.g., Dimian, 2003; Seider et al., 2004). One of the most appealing features of this heuristics-based approach is to decompose the seemingly complex task into a number of smaller tasks. Naturally, tackling several smaller problems is less formidable than taking on a large problem all at once. In contrast to the traditional horizontal decomposition (based on process units), this approach hierarchically decomposes the problem based on the control and operational objectives while ranking the most important one at the top and the least important one towards the end.

On the flip-side, due to the ever increasing complexity of chemical processes, any heuristics-based method is not self-sufficient, and over-reliance on heuristics is not advisable as the PWC decisions can, at times, be counter-intuitive or unconventional. For example, even in the case of a simple distillation column, unconventional control strategies, such as the use of feed temperature to respond to variations in feed compositions (e.g., Henry and Mujtaba, 1999), are possible. In addition, the ineffective usage of any heuristics-based approach by novice engineer(s), whose know-how is usually not adequate, may consequently result in inefficient control systems. Furthermore, heuristics cannot always be generalized and thus there is some degree of dissonance among researchers over the heuristics. For example, one of the guidelines in this heuristic-based approach proposed by Luyben et al. (1999) advocates to fix a flow in the recycle loop to avoid snowball effect. However, Larsson et al. (2003) claimed that this rule has a limited theoretical basis and cannot be generalized. Similarly, Larsson (2000) showed that this rule has bad self-optimizing properties and should not be applied for some processes.

Nonetheless, one of the captivating features of any heuristics-based method is that, they can strikingly simplify the complexity of the problem if used properly, which is the main reason for their wide-spread popularity. Hence, to round-out the only-heuristics-based methods, an integrated approach that pulls together the powers of rigorous simulation tools and heuristics is proposed in this study. The current simulation tools offer virtual hands-on experience and enhance process understanding. However, they cannot efficiently be used, especially for complex applications such as PWC, unless the user is conversant with them. So, one of the interesting advantages of this integrated approach is that the simulation tools can more effectively be used for plant-wide dynamic studies. Thus, both the heuristics and simulation tools get benefited by mutually sharing the strong traits of each through the integrated framework. Because of the importance and need to integrate heuristics with simulation tools, some simulation packages, such as BATCHES, are now coming up with open architectures wherein the user can add specialized heuristics into the simulator database (Watson et al., 2000). Due to the difficulty in obtaining rigorous models based on first principles, they have not extensively been used for PWC studies in the past. However, commercial process simulators like HYSYS and Aspen are now available, which can quickly develop first principles models with reasonable accuracy thus making the present study feasible. The present study used them extensively while designing the control system, whereas these tools have previously been used only to validate the resulting control system (but not to design the control system itself). As will be discussed in the later chapters, by making use of these tools in the early stages, one can design superior control systems.

In short, the scope here is to synthesize a generic procedure which can be used to develop an efficient plant-wide decentralized multi-loop control system, based on proportional-integral-derivative (PID) controllers, for a given process. Though advanced control technology has recently been witnessing rapid progress, decentralized control using PID controllers has been, and continues to be, the workhorse of the industrial control systems due to multiple reasons (Garelli et al., 2006): 1) simplicity in design and tuning, 2) ease of implementation, 3) more fault-tolerant, and 4) maintenance with less cost. Even for a model-based control system, PID control is often necessary at the base-level (Blevins et al., 2003) Thus, the success of model-based control depends on, up to certain extent, base-level PID control structure performance. Not getting the base-level control 'right' can cripple the overall control system. Furthermore, MPC is usually limited to one or a few units but not to the entire plant. This issue is discussed in detail in Chapter 7. In this regard, the present study, i.e., designing efficient base-level PID-based control structure, is still important even in the wake of advanced control technology.

Control Degrees of Freedom (CDOF) Procedure: CDOF is one of the foremost steps involved in any of the control system design as it tells the designer how many manipulated variables he/she has in order to control the process by regulating important process variables at their desired set-points. A new procedure to compute CDOF just based on basic qualitative knowledge of units in the process is proposed. The traditional, and also often tedious, analysis (i.e., to count all the equations and variables involved in the model) is not needed. Especially, when using process simulators for dynamic studies, it is a must to know the CDOF as it is not possible to control the process without placing the control valves. If the CDOF is not known, the designer might place less number of valves (which leads to an uncontrollable process) or more number of valves than required (e.g., one valve on each stream, which is not a good design practice as it leads to economically-less attractive process as additional valves incur more pressure drops). The feasibility of the proposed procedure is then demonstrated by successfully applying it to several processes whose complexity spans from low to very high.

Performance Assessment of PWC Systems: Due to the complexity of non-linear models and unavailability of non-linear model-based performance metrics, research in this field has largely been carried out using simplified/linear models and metrics based on them. However, the linear models are not always suitable and might introduce significant approximations in process dynamics, especially if the process is highly nonlinear. In addition, some of the earlier metrics are observed to be non-indicative of overall dynamic performance of the plant. Hence, a new metric is proposed which is applicable to both the linear and non-linear processes. This metric is named as ‘Dynamic Disturbance Sensitivity (DDS)’ as it characterizes the impact of disturbance on the process, and is defined as the sum of the absolute accumulation of all the components in the process. Using DDS as the measure, it is shown that the proposed control system performs as well as or better than the existing control structures in the literature.

Integrated Design and Control from Plant-Wide Perspective: Though integrated studies have received good attention in the recent past, these studies from plant-wide perspective are rather limited. The disadvantage of traditional sequential design and control approaches is that the design and control are carried out in two sequential steps, and the resulting design might be inoperable or unattractive from operations viewpoint. Whilst this problem can be resolved by optimization-based simultaneous approaches, they are often computationally intensive especially for large-scale problems (Zheng and Mahajanam, 1999). Hence, a modified sequential approach is presented by combining improved heuristics-based process design procedure and the proposed integrated framework for PWC.

Examples, based on industrial processes, are furnished to illustrate the feasibility and efficacy of proposed methods/tools for PWC, CDOF, performance assessment, and integrated design and control. Most of these illustrations are based on the hydrodealkylation (HDA) of toluene to produce the important petrochemical intermediate - benzene, which has been a standard test-bed for process design studies. Incidentally, benzene is the second most important intermediate for producing organic-based materials, and is used in the manufacture of well over 250 products such as ethyl benzene, cumene, cyclohexane and aniline. The HDA process is one of the processes to produce benzene from toluene, and also to produce quality naphthalene from suitable feed stocks (Liggin, 1997), thus signifying the industrial importance of the present study. Other ways to produce benzene from toluene include toluene-disproportionation (e.g., Nelson and Douglas, 1990) and toluene-steam dealkylation (e.g., Umeda et al., 1980). Though the HDA process has been used for design (e.g., Douglas, 1988) and control studies (e.g., Luyben et al., 1999; Qiu et al., 2003), in the present work, it has been more comprehensively studied. For example, several new process design alternatives using a membrane unit in the gas separation section are explored, and their economics and operation are assessed in this work. In addition, performance assessment of several PWC systems for the HDA process is carried out, besides developing a control system using the proposed framework.

1.3 Organization of the Thesis

This thesis has seven chapters. All the chapters are logically collated and the chapters are written in such a way that each one can be read independently. Following this chapter, Chapter 2 presents review of recycle dynamics and control, PWC methods and their systematic classification followed by importance of rigorous dynamic simulation tools. The integrated framework of simulation and heuristics, and its application are discussed in Chapter 3. A new procedure for CDOF and several applications are given in Chapter 4. The proposed dynamic performance measure (i.e., DDS) is discussed and then successfully used to evaluate the performance of several PWC systems in Chapter 5. Modified sequential approach for integrated design and control is presented in Chapter 6. Finally, conclusions and recommendations for the future work are given in Chapter 7.

CHAPTER 2

LITERATURE REVIEW AND SYSTEMATIC CLASSIFICATION OF PLANT-WIDE CONTROL METHODS*

Firstly, the importance of recycles in chemical processes is briefly discussed in this chapter. Review of recycle dynamics and control is then presented which eventually highlights the complexity involved in designing control systems for complex processes with multiple recycles. Following this, a review of several PWC methods proposed since early 1990s is presented. A more comprehensive collection of references on PWC methods is then systematically classified and tabulated, which would give a quick overview of existing methods and their important features. As discussed in the previous chapter, other relevant issues like CDOF, performance assessment, and integration of design and control are also studied in this thesis. Brief reviews on these topics are given in chapters 4, 5 and 6 respectively.

2.1 Recycles in Chemical Processes

Recycle streams are common in most of the chemical processes as it is not always possible to achieve complete (i.e., 100%) per-pass-conversion due to either thermodynamic limitations (e.g., in case of reversible reactions) or economic reasons (e.g., to improve the selectivity in case of complex reaction networks such as competing parallel reactions). With the increasing use of recycles, process complexity increases in terms of interaction among process variables, for example. Thus, though recycles are desirable from economics viewpoint, they are notorious for their ill-effects during control and operation of the plant. In the past, surge tanks were

* A preliminary version of this chapter was presented at the AIChE Annual Meeting, San Fransisco, USA, November 2003.

used to isolate the units and thereby reducing the interaction. However, surge tankage increases capital and operating costs due to additional inventory. Besides, at times, it is not advisable to keep the additional inventory for safety and environmental reasons, especially if hazardous chemicals are involved. Thus, there exists ample evidence to show that the increased interaction among various sections of the plant has become inevitable thereby entailing the need to study the dynamics and control of processes with recycles.

2.1.1 Recycle Dynamics and Control

Gilliland et al. (1964) were among the first to study the impact of recycles on dynamics, and they observed that recycles increase time constants of the process. Subsequently, Denn and Lavie (1982) showed that recycles increase the steady-state gain (i.e., increased sensitivity to disturbances) and the dominant plant time constant; another interesting observation is that the process exhibits increased sensitivity to low frequency disturbances. Kapoor et al. (1986) later observed that recycle severely affects the time constants of a high purity distillation column. In the following year, Papadourakis et al. (1987) demonstrated how recycle can affect Relative Gain Array (RGA), and showed that the RGA calculated for an individual unit can differ significantly from the actual RGA when the unit exists as a member of a complete plant.

Later, Luyben (1994) observed the snowball effect (i.e., small change in feed stream results in large changes in recycle streams) which is a typical characteristic of most of the processes with recycles. Morud and Skogestad (1994) noted that recycles may also cause instability or nonlinear behavior such as oscillatory (i.e., limit cycles) or even chaotic behavior. Morud and Skogestad (1996) observed that recycles, due to their feedback effect, affect poles of the system and thus possibly the stability; while parallel paths affect plant zeros and thus the achievable performance under feedback control. They also discussed less common, yet interesting, negative feedback effects of recycles. Mizsey and Kalmar (1996) showed that the recycle loop gain strongly influences the behavior and controllability of the process, while time constant influences somewhat less strongly. Jacobsen (1997) showed that recycles may introduce severe overshoots and inverse responses. Luyben (1998) introduced the term “external instability” to describe the phenomenon of destabilization due to recycles though the individual units are stable. Kumar and Daoutidis (2002) identified that recycle processes exhibit time-scale separation in their dynamics, i.e., the dynamics of individual units evolve in a fast time scale where the interactions are weak and the dynamics of the overall system evolve in a slow time scale where the interactions are significant.

Due to the aforementioned complex dynamic behavior of recycle systems, control system design for processes with recycles becomes relatively more challenging. Thus, several researchers addressed this issue. Taiwo (1986) proposed a recycle compensator to improve the control performance of single-input and single-output (SISO) processes, and later Taiwo and Krebs (1996) successfully extended it to multi-input and multi-output (MIMO) processes. In a series of papers, Scali and co-workers (Scali and Antonelli, 1995; Scali and Ferrari, 1997 and 1999) observed that the recycle compensator improves the control performance by counteracting the negative effects of recycle. Hugo et al. (1996) and Cuellar et al. (2005) presented techniques to develop approximate dynamic models of recycle systems for control purposes. Chodavarapu and Zheng (2001) provided a set of generic heuristics to design controllers for recycle systems, which require only a minimal amount of information on the recycle dynamics. Lakshminarayanan and Takada (2001) developed an empirical model of the recycle system and then designed a high performance recycle compensator. Later, Lakshminarayanan et al. (2004), using control loop performance assessment concepts, presented an index that gauges the severity of recycles thereby examining the need to implement (or not to implement) recycle compensator. Very recently, Tremblay et al. (2006) summarized the effects of recycles and detailed the benefits of recycle compensator.

2.2 PWC of Industrial Processes

Most of the studies in the previous section discuss the recycle dynamics and control of simple SISO systems with a single recycle. However, in reality, the plants contain dozens of unit operations with multiple recycles. Thus PWC is even more challenging. Foss (1973) posed the basic questions associated with PWC design: “Which variables should be controlled, which variables should be measured, which inputs should be manipulated, and which links should be made between them? It is a formidable task to sift from among these process variables those that should be measured and manipulated and to determine the control connections among them.” After around a decade, PWC was acknowledged as a creative challenge (Stephanopoulos, 1983). Since then, though there has been many works published on PWC, it still remains a challenge. For example, Stephanopoulos and Ng (2000) have recently stated that the synthesis of a control system for a chemical plant is an art; they further noted that the problem of PWC is “multi-objective” and so it is hard or impossible to solve it in a concise and rigorous manner.

Significant research has been initiated on PWC and, as a result, many PWC system design methodologies have been reported since 1964. The first PWC method is proposed by Buckley (1964) while the latest one is by Konda et al. (2005). Buckley (1964) proposed a PWC procedure that consists of two levels depending on frequency of disturbances. First, material balance control system is designed to handle vessel inventories for low-frequency disturbances. Product quality control system is then designed to regulate high-frequency disturbances. Konda et al. (2005) proposed an integrated framework consisting of heuristics and simulation tools. Though, PWC was initiated in 1964, PWC has been perused most actively only since early 90's and several PWC methods have been proposed during the last 15 years. In this section, some of these methods are briefly discussed chronologically while grouping similar methods (e.g., those proposed by same research group and any follow-ups or improvements). Comprehensive collection of various PWC studies is tabulated in the next section.

Price and Georgakis (1993) proposed a tiered framework in which control decisions are ranked based on their decreasing importance in order to arrive at a control structure that minimizes the propagation of disturbances. Later, Price et al. (1994), through dynamic simulation, suggested several guidelines for the throughput manipulator (TPM) selection and inventory control. Subsequently, this framework is used by Lyman and Georgakis (1995) to design a control structure for the TE process.

Narraway and Perkins (1993), based on linear dynamic models, presented a method to select the economically optimal control structure, and this method is further modified by Kookos and Perkins (2002). In their methodology, the objective is to maximize profit during transients resulting from upsets for a given plant design. Narraway and Perkins (1994) posed a mixed integer nonlinear optimal control problem (MINLP) to select an economically optimal multi-loop proportional-integral control structure. Lately, Kookos and Perkins (2001a) presented a heuristic-based mixed integer nonlinear programming (MINLP) in which the objective is to minimize the overall interaction and sensitivity of the closed-loop system to disturbances.

Turkay et al. (1993) presented a procedure using integer linear programming (ILP) and performance criteria such as internal model control interaction measure (IMCIM). IMCIM can be used to estimate the extent of influence of each manipulated variable (MV) on all control objectives. They have applied it to synthesize a regulatory control system for styrene plant using steady-state simulation package "PROCESS." However, they developed a control system for each individual unit operation separately using steady-state information and the dynamic simulation of the entire plant is not carried out.

McAvoy and Ye (1994) presented a PWC procedure by ranking the control loops based on time-scales to design a base-level regulatory control system for the TE process. This approach involves using a combination of steady-state screening tools, followed by dynamic simulation of the most promising candidates. Ye et al. (1995) suggested an optimal averaging level control and McAvoy et al. (1996) advocated a nonlinear inferential parallel cascade control to the control structure that was developed by McAvoy and Ye (1994) to improve its performance further. McAvoy (1999) presented a decentralized approach, based on steady-state (gain matrix) models and using optimization, to generate a base control system. His approach splits the synthesis into three stages: controlling safety variables in stage 1, production variables in stage 2 and the remaining process variables in stage 3. An optimization problem based on mixed integer linear programming (MILP), whose objective function is to minimize the absolute valve movement that is needed to mitigate the disturbance, is solved in each stage to select manipulated variables. Later, Wang and McAvoy (2001) extended this approach by including the dynamic models in the analysis; also, objective function is modified by including the sum of absolute values of the measured variable responses along with the sum of absolute valve movements, i.e., it involves the tradeoff between manipulated variable moves and area under the transient response curve of process variables. Lately, Chen and

McAvoy (2003) developed a new ‘optimal control’ based PWC method and applied it to vinyl acetate process. Chen et al. (2004) later extended this method to processes with multiple steady-states. Robinson et al. (2001) presented an “Optimal Control” based approach to design a decentralized PWC system. This approach is based on splitting the optimal controller gain matrix that results from an output optimal control problem into diagonal feedback and off-diagonal feedforward components which are then used to design and evaluate decentralized control systems. Based on these results, they observed that the pairing resulting from steady state RGA is not always reliable. They got a significantly different pairing whose performance is comparable with that of MPC.

Banerjee and Arkun (1995) presented a systematic mathematical approach called control configuration design (CCD), to design a decentralized PWC structure. It is a two-tiered procedure based on time-scales. In the first tier, control structure for pressure, level and temperature are considered while compositions are considered in the second tier. They have also discussed issues like insufficient modeling information, complexity and poor knowledge of effective bounds on model uncertainties and disturbances. Major steps involved in their procedure are:

a. Selection: choosing a subset of controlled variables and manipulated variables based on the necessary condition for robust stability.
b. Partitioning: considering all the possible pairings for the subset of controlled variables that made it past selection and testing them for
    i. Nominal stability – the candidate configuration must be nominally stable.
    ii. Small cross feed performance degradation – the candidate configuration should not suffer much performance degradation as a result of decentralization.

Qiu et al. (2003) later successfully applied the CCD approach to the HDA process.

Ricker and Lee (1995) developed a plant-wide nonlinear model predictive controller (NMPC) for the TE process. Later, Ricker (1996) designed a decentralized control strategy for the TE process by employing heuristics and compared its performance with NMPC. He noted that the decentralized control outperforms NMPC for such a complex and nonlinear process.

Ng and Stephanopoulos (1996) proposed a hierarchical framework, multi-horizon control system, in which the plant is vertically decomposed into a set of representations of different degrees of abstraction. This methodology consists of two phases based on time horizon:

a. Phase I : Long-horizon Analysis.
b. Phase II: Short-horizon Analysis.

In each of these phases, a control strategy has to be developed to satisfy the control objectives according to their prioritization. Starting from the simple input-output level (the longest time-horizon) of representation, this step has to be repeated until we reach the most detailed level of representation which models the shortest time-horizon of operation in the plant. The control objectives and the control strategy have to be refined in each level. Stephanopoulos and Ng (2000) suggested guidelines for the prioritization of the control objectives, which is one of the important steps involved in PWC system design.

Samyudia et al. (1996) have proposed a PWC method based on decomposition of the plant into smaller sections and then designing the control system for each section. The decomposition is based on “gap metric” concept with the aim to minimize the interaction among different sections. Decomposing the plant into several sections, each one with a single unit, is shown to be inferior to decomposing the plant into sections consisting of one or more units. Later, a more generalized version of this method is proposed by Lee et al. (2000).

Cao et al. (1996 and 1997) and Cao and Rossister (1997) presented several mathematical tools that aid in the initial screening and selection of PWC structure, some of which are similar to the other measures like Relative Disturbance Gain (Stanley et al., 1985).

a. Cao et al. (1996) presented two open-loop analysis techniques, based on modified singular value analysis (SVA) and optimization based approach, for assessing input-output controllability in the presence of control constraints. Cao et al. (1997) later proposed two input screening techniques for effective disturbance rejection in the presence of manipulated variable constraints: (1) Worst Case Input-Disturbance Gain (WCIDG) and, (2) Input-Disturbance Gain Deviation (IDGD).
b. Cao and Rossister (1997) proposed a pre-screening technique called Single-Input Effectiveness (SIE) for selecting manipulated variables having the largest effect on controlled variables, from a range of possible control inputs by eliminating ineffective inputs. Cao and Rossister (1998) proposed a new measure, the input disturbance alignment (IDA), to identify the set of manipulated variables from a large number of candidate inputs which can effectively reject localized disturbances.

Luyben and co-workers (Luyben et al., 1997; Luyben et al., 1999) proposed a more comprehensive 9-step heuristic procedure and applied it to several industrial case-studies. This is a hierarchical procedure which ranks the control and operational objectives based on their importance.

Semino and Guiliani (1997) proposed a systematic steady-state analysis procedure, Snowball Effect Analysis (SEA), which is able to analyze all possible control configurations and order them according to their ability to reject disturbance(s) without saturation of the manipulated variables i.e., classify them into two classes based on whether a particular structure is affected or not affected by snowballing.

Zheng et al. (1999) proposed a hierarchical procedure for synthesizing optimal PWC system in which alternative configurations are compared based on (steady-state) economics. The controllability aspects are also taken into consideration by introducing a cost index associated with dynamic controllability.

Jorgensen and Jorgensen (2000) presented a procedure in which the control structure selection problem is formulated as a MILP, employing cost coefficients which are computed using Parseval's theorem (Riley et al., 2002).

Skogestad (2000a and 2000b) presented a procedure to design a self-optimizing PWC system. The main idea is to identify suitable controlled variables, which when kept at constant set-points, lead to near-optimal operation with acceptable loss in the presence of disturbances. His analysis is mainly based on steady-state models as the economic performance is primarily determined by steady-state considerations. However, he partly included the dynamic performance by considering a control error term as an additional disturbance. The main steps that are involved in his procedure are degrees of freedom (DOF) analysis, definition of optimal operation, and evaluation of loss when the controlled variables are kept constant rather than optimally adjusted. An expanded version of this procedure is later presented by Skogestad (2004) by including the issues such as inventory and production rate control.

Zhu et al. (2000) proposed a hybrid PWC strategy based on integrating linear and nonlinear MPC. This hybrid method is applicable to plants that can be decomposed into approximately linear subsystems and highly nonlinear subsystems that interact via mass and energy flows. They proposed a simple controller coordination strategy that counteracts interaction effects for the case of one linear and one nonlinear subsystem. Later, Zhu and Henson (2002) applied this strategy to styrene plant.

Rodriguez and Marcos (2002) developed an expert system which can generate a PWC structure for the TE process. This expert system has been programmed using CLIPS, an expert system tool developed by the Software Technology Branch, NASA/Lyndon B. Johnson Space Center. They applied this approach to some other industrial processes and got valid control structures. This expert system is composed of three independent modules:

a. Module I: Topology of the plant and information about components and reactions.
b. Module II: Control Objectives.
c. Module III: Control Heuristics.

Vasbinder and Hoo (2003) have proposed a decision-based approach. A modified analytical hierarchical process (mAHP) is used to decompose the entire plant into smaller modules and then the 9-step heuristic procedure of Luyben et al. (1999) is used for each module to develop PWC system. Later, Vasbinder et al. (2004) used this decision-based approach to design PWC system for the HDA process.

In addition to the several research articles reviewed above, lately, PWC has even appeared as a new topic in the revised versions of standard design and control text books (Bequette, 2003; Seider et al., 2004; Seborg et al., 2004); and there is a more advanced textbook by Luyben et al. (1999) which is almost exclusively devoted to PWC.

2.3 Systematic Classification of PWC Methods

From the above section, it is evident that many different PWC system design methodologies, which are capable of designing PWC systems of various types ranging from decentralized to centralized control strategies, are available. However, so far, very limited attention has been paid towards the systematic classification of these methodologies. Most of the times, the PWC system designer may not be aware of all the available methodologies and their features. A systematic classification is desirable in order to have an overall picture of various methodologies which would in turn lead to better understanding and improved methodologies. Thus, various PWC system design studies are classified here in two ways. The first classification is based on the main approach in the method (approach-based classification in Table 2.1) and the second classification is based on the controller structure adopted (structure-based classification in Table 2.2). Approach and structure are attributes for all the methodologies and thus form a good basis for classification.

One recent attempt towards the classification of PWC methodologies is by Larsson (2000). However, classifications in Tables 2.1 and 2.2 are more comprehensive and up-to-date. Larsson (2000) addressed only the decentralized control strategies but not the centralized control strategies. Structure-based classification in Table 2.2 includes the centralized control strategies as well. In addition, many recent methodologies, which were not in the Larsson's classification, have been included in Tables 2.1 and 2.2. Usually, the mathematical and optimization approaches are considered alike. However, keeping in view the large number of such methodologies and the differences in techniques employed in them, they are classified separately as mathematical and optimization approaches in Table

2.1. The mathematical approaches use process models (steady-state and/or dynamic) along with controllability tools like *relative gain array (RGA), Niederlinski index (NI), singular value decomposition (SVD), condition number (CN), disturbance condition number (DCN), closed loop disturbance gain (CLDG), relative disturbance gain (RDG), performance relative gain (PRG)* etc. On the other hand, optimization approaches use numerical methods like *MILP, MINLP* etc. In this regard, these two approaches are classified into two different classes.

Classification of PWC system design methodologies is challenging as some of them might fit into more than one category since they adopt a few approaches and/or structures. Thus, the subdivisions cannot be considered to be mutually exclusive. For example, multi-horizon control system of Ng and Stephanopoulos (1996) employs a hierarchical framework in which the plant is vertically decomposed into a set of representations of different degrees of abstraction. Starting from the longest time-horizon of operation (input-output structure), they try to identify and prioritize the significant control objectives in that representation of the plant, and then a control system is designed to satisfy these objectives according to their priority in that level. They then move down to one level of the hierarchy to refine the model and correspondingly the objectives and control system in order to meet the overall plant objectives in that shorter time-horizon of operation. This procedure is repeated till the shortest time-horizon of operation is reached. Therefore, the methodology of Ng and Stephanopoulos (1996) can be placed in the vertical decomposition based on process structure or in the vertical decomposition based on control objectives in Table 2.2. We opted to put this methodology in the former as it places greater emphasis on vertical decomposition based on process structure. Nevertheless, these subdivisions provide convenient means to classify various PWC methodologies. Through these classifications, researchers and engineers can immediately identify the two main features of any PWC methodology at a glance. It should be noted that, in addition to the references that propose PWC methods, references that merely apply the proposed methods are also included in these classifications; these applications (e.g., Lyman and Georgakis (1995); Qiu et al. (2003); Vasbinder et al. (2004)) demonstrate the general validity of the respective methods and also offer greater insight.

Table 2.1: Approach-Based Classification of PWC System Design Methodologies

Approach	Methodology*
Mathematical (model oriented) approaches	Banerjee and Arkun (1995), Cao et al. (1997), Cao and Rossister (1997 & 1998), Groenendijk et al. (2000), Dimian et al. (2001), Herrmann et al. (2003), Qiu et al. (2003)
Heuristics (process oriented) approaches	Govind and Powers (1982), Newell and Lee (1989), Ponton and Laing (1993), Price and Georgakis (1993), Price et al. (1994), Lyman and Georgakis (1995), Ricker (1996), Luyben et al. (1997), Luyben et al. (1999), Riggs (2001), Konda et al. (2005)
Optimization (algorithmic) approaches	Morari et al. (1980), Narraway and Perkins (1993 & 1994), Ricker and Lee (1995), Kanadibhotla and Riggs (1995), Semino and Giuliani (1997), Zhu et al. (2000), Zheng et al. (1999), Heath et al. (2000), Kookos and Perkins (2002), Zhu and Henson (2002), Meadowcroft et al. (1992)
Artificial Intelligence (e.g., expert systems, neural network) based approaches	Rodriguez and Marcos (2002), Conradie and Aldrich (2001)
Mixed approaches	Buckley (1964), Umeda et al. (1978), Douglas (1988), Turkay et al. (1993), Fonyo (1994), McAvoy and Ye (1994), Ng and Stephanopoulos (1996), Samyudia et al. (1996), Lausch et al. (1998), McAvoy (1999), Jorgensen and Jorgensen (2000), Larsson (2000), Lee et al. (2000), Skogestad (2000a, 2000b and 2004), Kookos and Perkins (2001a), Robinson et al. (2001), Wang and McAvoy (2001), Castro and Doyle (2002 and 2004), Chen and McAvoy (2003), Vasbinder and Hoo (2003), Chen et al. (2004), Seborg et al. (2004), Vasbinder et al. (2004)

*Methodologies in each sub-group are arranged chronologically.

Table 2.2: Structure-Based Classification of PWC System Design Methodologies

<table>
<tr><th>Structure</th><th>Basis</th><th colspan="2">Methodology*</th></tr>
<tr><td rowspan="5">Decentralized (Multi-loop SISO) strategies</td><td>Horizontal decomposition based on process units</td><td colspan="2">Umeda et al. (1978), Turkay et al. (1993)</td></tr>
<tr><td rowspan="3">Vertical decomposition based on hierarchy</td><td>Decomposition based on process structure</td><td>Morari et al. (1980), Ponton and Laing (1993), Ng and Stephanopoulos (1996), Samyudia et al. (1996), Lee et al. (2000), Vasbinder and Hoo (2003), Vasbinder et al. (2004)</td></tr>
<tr><td>Decomposition based on control objectives</td><td>Newell and Lee (1989), Price and Georgakis (1993), Price et al. (1994), Lyman and Georgakis (1995), Ricker (1996), Luyben et al. (1997), Luyben et al. (1999), McAvoy (1999), Riggs (2001), Wang and McAvoy (2001), Rodriguez and Marcos (2002), Chen and McAvoy (2003), Chen et al. (2004), Konda et al. (2005)</td></tr>
<tr><td>Decomposition based on time scales</td><td>Buckley (1964), Fonyo (1994), McAvoy and Ye (1994), Banerjee and Arkun (1995), Lausch et al. (1998), Qiu et al. (2003)</td></tr>
<tr><td>Miscellaneous</td><td colspan="2">Govind and Powers (1982), Douglas (1988), Narraway and Perkins (1993 & 1994), Semino and Giuliani (1997), Cao et al. (1997), Cao and Rossister (1997 & 1998), Zheng et al. (1999), Jorgensen and Jorgensen (2000), Larsson (2000), Heath et al. (2000), Groenendijk et al. (2000), Skogestad (2000a, 2000b and 2004), Dimian et al. (2001), Kookos and Perkins (2001a & 2002), Seborg et al. (2004)</td></tr>
<tr><td rowspan="3">Centralized (Multivariable MIMO) strategies</td><td>Linear model</td><td colspan="2">Meadowcroft et al. (1992)</td></tr>
<tr><td>Nonlinear model</td><td colspan="2">Herrmann et al. (2003), Conradie and Aldrich (2001)</td></tr>
<tr><td>strategies based on both linear and nonlinear models</td><td colspan="2">Zhu et al. (2000), Zhu and Henson (2002)</td></tr>
<tr><td>Mixed strategies</td><td colspan="3">Ricker and Lee (1995), Kanadibhotla and Riggs (1995), Robinson et al. (2001), Castro and Doyle (2002 and 2004)</td></tr>
</table>

* Methodologies in each sub-group are arranged chronologically.

2.4 Dynamic Modeling and Process Simulators

Control engineers have been using dynamic simulation tools over decades to study process control concepts and to design control systems. Dynamic models for some standard unit operations are given in several text books (e.g., Luyben, 1990). Most of the control studies in the past, however, are based on linear models and/or individual units. Watson et al. (2000) nicely discussed the problems associated with decisions based on individual unit simulations, and subsequently highlighted the need to carry out plant-wide simulations based on a case-study that involves retrofitting a pharmaceutical plant. However, as stated by Mandler (2000), though SIMULINK can efficiently handle small scale problems, it is too cumbersome to use SIMULINK for plant-wide simulations; thus, process simulators, such as SPEEDUP, are more suitable for PWC studies.

Process simulators have a wide range of applications spanning from process control, operation, troubleshooting and training (Sowa, 1997). For example, Feliu et al. (2003) have recently demonstrated how such simulators can improve product quality, productivity and process safety. In addition, they can also be used in startup studies (e.g., Fabro et al., 2005) and in process optimization (e.g., Jang et al., 2005). However, despite the expected benefits of these simulators, as stated by Marquardt (1991), they have not widely been used in the process industry due to several reasons; one of the main reasons being the significant effort and time needed to setup and analyze rigorous dynamic models. The situation is slowly changing due to the advancements in computing technology, object-oriented programming and numerical methods; and these dynamic simulation tools are evolving into a tool for everyday use by engineers. Consequently, several dynamic simulation tools, both in-house and commercial, are now available. For example, Cole and Yount (1994) demonstrated the use of in-house simulation tools to develop and analyze control and safety systems for industrial processes. Longwell (1994) presented three projects that have resulted in millions of dollars of economic benefit by improving the plant operability using DuPont's in-house simulator, TMODS.

Since early 90's, several commercial dynamic process simulators (e.g., Aspen Dynamics, HYSYS) are available with reasonably sophisticated features. Laganier (1996) presented some applications using commercially available simulation packages including SpeedUp, HYSYS, Winsim and gPROMS, and discussed their capabilities and shortcomings. Since then, these simulators have been gradually improved to become more accurate, robust and user-friendly, and these improvements are expected to continue due to the continuing research effort in this direction. For example, most of the existing process simulators are based on differential algebraic equations (DAE). Over the last decade, there has been increasing attention towards integrating partial differential algebraic equations (PDAE) in such simulators to further the modeling accuracy (e.g., Oh and Pantelides, 1996; Martinson and Barton, 2000). Similarly, simulation tools that can support both the continuous and discrete systems are becoming available (e.g., Rodriguez, 2005).

Several applications of HYSYS and Aspen Dynamics for control of industrial processes are discussed by Luyben (2002), while Seider et al. (2004) discussed how these simulators can be used in process design, control and optimization. Another notable and one of the most recent dynamic simulation packages is "ForeSee" (Tu and Rinard, 2006). ForeSee differs from most of the existing dynamic simulators in the way the equipment models are represented. Existing process simulators model the standard unit operations. On the other hand, ForeSee has four component models -

containments, core models, connectors, and coordinators – which can be combined to model/simulate standard unit operations. For example, instead of a distillation column model, ForeSee contains a model of a more fundamental component, i.e., tray, and such tray models can then be assembled to generate model for a distillation column. In addition to all the above-mentioned simulation packages, industry-specific process simulators are also available in order to address particular needs of different process industries; for example, Polymer Plus and RefSYS can be used to simulate polymer processes and refineries, respectively. Similarly, simulation packages, such as BATCH-DIST (Diwekar and Madhavan, 1991), are available to simulate multi-component batch distillations. Lately, Barrero et al. (2003) discussed the development and testing of simulation models for power plants, and Chen and Adomaitis (2006) presented simulation models for semiconductor processes.

Despite the increasing availability of the dynamic process simulators, their usage in PWC research is rather limited. Out of the many PWC studies presented in the previous section, only a few are carried out using such rigorous simulators, and thus the PWC community has not fully explored the power of these simulators. Prompted by these observations, in this thesis, a commercial process simulator (i.e., HYSYS) is extensively used to model the HDA process in all the illustrations. HYSYS has many standard unit operations which are developed using first-principles based models. Though some standard units, such as rate-based distillation column, membrane and fluidized bed reactor, are not available in HYSYS, they can be easily modeled using Visual Basic. Besides, thermodynamic properties (such as vapor-liquid equilibrium) can be predicted using an extensive collection of traditional property packages, such as Peng-Robinson (PR) and Non-Random-Two-Liquid (NRTL) equations. If the database is not available to make use of these methods (e.g., if the binary interaction parameters are not available), newer ones such as conductor-like screening models (COSMO) are now becoming available which can predict thermodynamic properties based on solvation thermodynamics and computational quantum mechanics (Mullins et al. 2006). However, the thermodynamic properties for the components in a conventional petrochemical process such as the HDA process can be predicted with reasonable accuracy using the PR model in HYSYS (e.g., Peng and Robinson, 1976); hence, PR model is used in the present study.

2.5 Summary

Considering the importance and complexity of recycle systems, significant research has been carried out on recycle dynamics since early 1980s. Following this, control of recycle systems has been given great deal of attention since late 1980s. Subsequently, the control of more complex systems (i.e., control of plants with several recycles - PWC) has been one of the active areas of research in the last 15 years. Due to the availability of a large number of PWC methods, comprehensive and systematic classifications are presented in this chapter from which researchers can easily identify the two important features (i.e., the approach used and the structure employed) of each method. From Table 2.2, it is evident that relatively more number of methods based on decentralized multi-loop SISO strategy are available when compared to the number of methods based on its counterpart, i.e., centralized control strategy; this is mainly due to the complexity involved in applying the latter to large scale processes. From Table 2.1, artificial intelligence (AI) based approaches for PWC are rather limited. However, such approaches can be expected to be available in future due to increasing applicability of AI techniques.

Despite the availability of powerful process simulators, these have not extensively been used by PWC community. Thus, in this thesis, a commercial process simulator (i.e., HYSYS) is used to explore and evaluate its potential for PWC studies. In addition to PWC, other relevant issues like performance assessment of PWC systems and interaction between design and control from plant-wide perspective are also studied in Chapters 5 and 6 respectively. Brief review of the literature pertaining to these topics is given in the respective chapters.

CHAPTER 3

INTEGRATED FRAMEWORK OF SIMULATION AND HEURISTICS*

More effective and efficient PWC methodologies are becoming increasingly important as chemical processes are becoming more and more integrated with recycles for reasons of safety, environmental considerations and economics. Hence, in this chapter, an integrated framework of simulation and heuristics is proposed. The main emphasis here is on vertical integration of simulation and heuristics which exploits the inherent interlink between them. By adopting this framework, simulators can be more efficiently utilized and they also offer invaluable support to the decisions taken by heuristics. The proposed framework is then successfully applied to the HDA process. An analysis of results shows that the proposed framework builds synergies between the powers of both the simulation and the heuristics thereby resulting in a practical PWC methodology that leads to a viable control system.

3.1 Introduction

Plant-Wide Control: In the past, unit-based control system design methodology (Umeda et al., 1978) has been widely used to design control systems for complete plants. However, the recent stringent environmental regulations, safety concerns and economic considerations, demand the design engineers to make the chemical processes highly integrated with material and energy recycles. As discussed in Chapter 2, several researchers studied the effect of these recycles on the overall dynamics and concluded that recycles need special attention while

* This chapter is based on the paper - Konda, N. V. S. N. M.; Rangaiah, G. P.; Krishnaswamy, P. R. Plant-Wide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics. Ind. Eng. Chem. Res. 2005, 44, 8300-8313.

designing PWC systems as they change the dynamics of the plant in a way which may not always be apparent from the dynamics of the individual unit-operations. Hence, the unit-based methodology seems to be scarcely equipped to design the control system for such complex plants. For example, Downs (1992) reported a control strategy for a scrubber-distillation column with a liquid recycle which did not work from an overall point of view, though the control of individual unit operations was satisfactory. Luyben (2000a) also demonstrated how control decisions vary based on perception i.e., whether the unit is considered as a single unit-operation or an integral part of the plant. Thus, there is a need for better methodologies which can deal with the highly integrated processes in a more efficient way. This leads to the concept of PWC which demands plant-wide perspective while designing PWC systems.

Designing control systems for highly integrated processes is challenging because of the large combinatorial search space. For example, Price and Georgakis (1993) observed 70 alternative control strategies for a simple hypothetical reactor-separator process with a single recycle. Keeping in view of this large combinatorial search space, the ultimate solution may not be so intuitively obvious. So, many researchers have addressed PWC problem over the last two decades and came up with various methodologies. After a critical review of various methodologies, the heuristic-based methodologies are found to be easier not only to understand but also to implement. However, novices often face difficulties while adopting some of these heuristics which need experience and basic process understanding for their effective usage. This problem can be best addressed by using simulation tools such as HYSYS, which are becoming increasingly popular and can give “virtual hands-on experience” to novices. Moreover, heuristics cannot always be totally relied upon as the solution can sometimes be unconventional. In addition, heuristics can sometimes be contradictory and leave the designer in a dilemma (Douglas, 1985). Motivated by these, we integrated simulation tools and heuristics to develop a simulation-based heuristic methodology which can handle the PWC problem effectively and realistically.

Chemical Process Simulators: Although simulation tools have seen widespread usage in process control related applications in the past, most of these studies are based on steady state simulation and a few of them are based on dynamic simulation of individual unit operations with little emphasis on PWC (Tyreus, 1992). It is only around early 1990s that the advent of computer technology permitted the development of commercial plant-wide dynamic simulators. Since then, the field of dynamic simulation is rapidly growing and, today, several commercial dynamic simulators, such as HYSYS Dynamics, which can effectively model large-scale processes, are available. However, even with the present day advances, using dynamic simulators, especially for complex applications such as PWC system design, is not easy. It is just not enough to know the simulators per se. It demands more than that along with the application of solid engineering principles and significant amount of time. These issues are much more pronounced especially in the context of PWC. So, integrating the PWC heuristics with the dynamic simulation capabilities, as discussed in this chapter, greatly facilitates the PWC system design and increases use of dynamic simulation.

Some design heuristics and simulation techniques have already evolved as integrated tools and some of the process design studies are being carried out using simulators along with the aid of heuristics which proved to be very beneficial. For example, a designer can save time if the design heuristic: *keep the operating reflux ratio at 1.2 times the minimum reflux ratio* is known. Else, the designer would have to explore a larger search space to find the optimal solution. Applying this heuristic certainly makes the designer's task easier while simulating and optimizing distillation columns.

Most of the single unit operation control studies can be done fairly easily by using dynamic simulation tools. But, the complexities associated with dynamic simulation tools precluded the application of these tools especially to PWC problems. Thus, rigorous nonlinear simulation was used in a few studies only to evaluate/validate the control systems once they are developed. However, the recent technological advances made the simulation technology mature enough to handle even the complex problems within a reasonable amount of time (Sowa, 1997). Moreover, Moore's law states that the computing speed doubles every 18 months which in turn nurtures progress in the simulation technology. Hence, simulators are likely to gain widespread use throughout the process industries and in academia. With the promise of these improvements in the simulation technology, the PWC community can benefit by addressing PWC problems with the aid of the simulation tools.

The remaining chapter is organized as follows: the next section presents an integrated framework of simulation and heuristics for PWC of industrial processes. Section 3.3 includes the details of the HDA process and its steady-state modeling using HYSYS. Application of the proposed methodology to the HDA process and the resulting control systems' performance evaluation are presented in section 3.4. Finally, chapter summary is given in section 3.5.

3.2 Proposed Integrated Framework of Simulation and Heuristics

The objective of this section is to develop a unified PWC methodology which is amenable to study practical concerns in a flexible way which in turn would lead to the best-practical solution (control system). After a careful review of PWC methodologies, heuristic-based methodologies are found to be intuitively attractive because they are easier to understand and implement. Heuristic-based methodologies just need the basic understanding of the process along with some experience. So, we have chosen to develop a heuristic-based methodology. Mathematical tools such as RGA are also used, wherever necessary, to reap more benefits. Pioneering work in this direction is by Luyben et al. (1999) who proposed a 9-step heuristic procedure. This procedure will be referred as Luyben's methodology hereafter. While this methodology does not have any serious limitations, it does have some shortcomings. For example, Luyben et al. (1999) sub-divided the big task of designing the overall PWC system into smaller tasks. However, in each step (especially set production rate and material inventory steps) the decision is ad hoc, which would impede the usage of this methodology. As the TPM dictates the overall control system structure and thereby performance, the production rate must be set carefully. To make the situation worse, production rate is a typical kind of variable for which one can find many alternatives. Moreover, overall material inventory control is obviously a plant-wide concern as it must be a self-consistent structure (Price and Georgakis, 1993). Though a general discussion is given in Luyben et al. (1999) specific guidelines are not apparent from this discussion. Systematic guidelines at this stage are essential. So, we adopted the guidelines from Price and Georgakis (1993) to facilitate the selection of manipulators for the throughput and inventory regulation.

One of the heuristics in Luyben's methodology is to fix a flow in the recycle loop to avoid snowball effect, which is popularly known as Luyben's rule. It gives an impression that the flow in the recycle loop has to be controlled whenever there is a recycle. But this need not always necessarily be true. For example, the proposed integrated framework develops a viable control system (discussed in section 3.4) which does not require any flow control in the recycle loop. Similar observation was made by Bildea et al. (2000) and Dimian (2003). The former formulated a mathematical criterion based on which one can judge when the conventional control structure can perform better than the control structure developed by applying Luyben's rule. Dimian (2003) presented some cases wherein the conventional control structure can perform better than the control structure developed by applying Luyben's rule. Balasubramanian et al. (2003) showed that fixing a flow in the recycle loop can result in instabilities especially when there are delays which are often the case in reality. Moreover, snowball effect cannot really be eliminated from the process by fixing a flow in the recycle loop but it is only transferred from one location to another (Yu, 1999). So, better alternatives to avoid snowball effect rather than fixing flow in the recycle loop are needed.

Though Luyben's methodology (1999) yields viable control structures, some of them are 'unbalanced'† control structures which are not desirable. In addition to this, Luyben's methodology may yield "self-inconsistent" structures (self-consistency is discussed in Appendix A). Though these structures may be workable control strategies, extensive simulation studies by Price and Georgakis (1993) have shown that they are inferior to self-consistent structures in terms of performance. There are other issues (especially in complex integrated processes) that are not intuitive. As

† If there is any disturbance affecting the process, flow rates of all streams in the process will have to vary according to material balances. But, fixing a flow in the recycle loop forces the control system to act on the system to reach a forced steady state in which one or more units need to take more rigorous action than others. This kind of control structures is called unbalanced control structure (Yu, 1999).

these issues can be best addressed by dynamic simulation, dynamic simulation and heuristics are integrated to find a practical solution. In every level/stage, nonlinear steady-state and dynamic models of the plant are used to take the decision or to support the decision suggested by heuristics. A few reported studies on PWC are based on steady-state models. One of the major downsides of these methodologies is that the steady-state feasibility of the process does not guarantee the plant-wide controllability. In addition, steady-state analysis might not be adequate for control studies all the time (Skogestad and Jacobsen, 1990). So, dynamic simulation should be more emphasized especially in the context of PWC.

The improved heuristic methodology consists of eight levels (Table 3.1). Various steps involved along with the *role of simulation models* in each step of the methodology are discussed below.

Level 1:

Define PWC Objectives: PWC objectives should be formulated from the operational requirements of the plant. These control objectives typically include product quality, production rate, stable operation of the plant, process and equipment constraints, safety concerns and environmental regulations. Many a times, there can be disagreement between the plant-wide objectives and unit operations objectives. For example, the best local control decisions (in the context of single units), may have long-range effects throughout the plant (Stephanopoulos and Ng, 2000). In this case, the plant-wide objectives should be given priority as ultimately the plant as a whole should operate properly. Considerable attention need to be paid while defining the PWC objectives as the control system decisions are dictated more by the underlying operating objectives than the control performance (Downs, 1992).

Role of Simulation Models: All the objectives can be set by process requirements. Coming to the objectives related to the process stability, the question at this stage is whether the process is operating at stable steady-state or not. This can be answered by the steady-state and dynamic simulation models. For example, in the case of feed effluent heat exchanger with a plug flow reactor, the steady-state simulation model with and without energy recycle can be perturbed to see whether it is converging to the same values in both the cases. If so, one can conclude that the process is operating at stable operating conditions; otherwise, the process is operating at unstable steady-state. Dynamic simulation models can also be used to check whether the process is stable or not (i.e., by checking the process variables' responses are bounded or not). The dynamic stability is guaranteed later in Level 4.

Determine CDOF: Luyben et al. (1999) proposed to count the number of control valves to find the CDOF of the process. This is true but not a practical solution at this stage because, many a times, it is the job of the control engineer to place the control valves in the process flow diagram which needs the knowledge of CDOF of the process. That means the CDOF is a priori information that needs to be known before the placement of control valves. Accordingly, control valves can be placed in strategic locations in the plant. Else, it may so happen that more or less control valves may be placed if the engineer is not familiar with the plumbing rules. These kinds of problems occur more frequently if the process is highly integrated. If more valves are placed, the process would be less economical due to the increased power requirements for compressors and pumps. On the other hand, if fewer valves are placed, all the control objectives cannot be achieved or, at times, the process can even become uncontrollable.

Traditionally, CDOF is obtained by subtracting the sum of number of equations and externally defined variables from the number of variables (Seborg et al., 2004; Seider et al., 2004). This procedure is impractical for highly integrated plants and prone to error (Seborg et al., 2004, p. 238). Ponton (1994) proposed a method for CDOF by counting the number of streams and subtracting the number of extra phases (i.e., if there are more than one phase present in that unit). However, simple examples can easily be constructed where this method fails. For example, CDOF for a heater/cooler remains the same irrespective of the number of phases involved in the unit. Larrson (2000) also observed some cases wherein Ponton's (1994) method fails. So, a simpler and accurate procedure to calculate the CDOF will be more useful; such a procedure is proposed and discussed in detail in Chapter 4. For the time being, it is assumed that the information about CDOF is available (e.g., by counting the number of valves in the process).

Level 2: Unlike many works, full PWC system design problem including the parametric decisions (tuning parameters) is addressed here. Hence, the following issues are mandatory.

Identify and Analyze Plant-Wide Disturbances: It is important to have a notion about the nature of disturbances expected along with their sources, magnitude and also how they propagate through the plant as they have considerable impact on the selection of control structure (Moore, 1992; Price and Georgakis, 1993; Marlin, 1995) and controller tuning. For example, Price and Georgakis (1993) observed different control structures performing differently for different disturbances.

Role of Simulation Models: Expected disturbances can be tried out on the steady-state simulation model to observe how the effect of the disturbances is propagating throughout the plant; While trying out various disturbances on the steady-state simulation model, one must make sure that the specifications given are appropriate. This analysis would be useful later while tuning the controllers. For example, anticipated disturbances can have more severe effects at some sections of the plant and hence the controllers in these sections should be tuned more conservatively to make all the sections of the plant equally robust. This is one of the important requirements that arises from plant-wide perspective, and is confirmed from our extensive simulations - the most sensitive sections in the plant required relatively more conservative tuning for good rejection of the disturbances studied.

Set Performance and Tuning Criteria: This step should be considered before any structural/parametric decisions as performance criteria have considerable impact on structural/parametric decisions. For example, Price et al. (1994) showed that control structure may differ with the performance criteria chosen. Setting an unanimous performance criterion for the overall plant control system is a challenging task as there can be many loops of different dynamics. For example, one would prefer quick settling for fast-responding loops like levels and will go for P-only controllers where off-set is not very important. On the other hand, one would prefer zero offset for slow-responding loops like composition. To make the situation worse, it is not only the kind of loop but also the location of the loop also dictates the performance criteria. For example, in the case of level control, one cannot always go for averaging control; one will have to go for less conservative tuning if the level is in a distillation column and the performance criteria would also depend on the control structure selected. Control structure for distillation bottoms composition and reboiler level is a good example wherein the performance criteria change with the control structure considered; if the column base level is controlled by reboiler heat input and bottoms composition is controlled by bottoms flow, then the level control should be tightly tuned since it is nested inside the composition loop which otherwise would have been tuned conservatively (Luyben, 2002).

Performance criteria such as integral error can be considered but analysis would be much more difficult. Hence, in the preliminary stages, settling time (not the normalized settling time is used in the initial screening stage; more rigorous analysis is carried out during the final selection of control system, as will be discussed in chapters 5 and 6) is considered as the performance criterion (while making sure that all the process objectives and constraints are satisfied) for highly complicated processes with dozens of control loops involved. Integral error can be chosen as the performance criterion for more rigorous studies in later stages. Performance assessment of PWC systems is the subject of Chapter 5; and a measure to gauge the plant-wide dynamic performance based on rigorous and nonlinear simulation is proposed in Chapter 5. As the improved heuristic methodology is integrated with dynamic simulation, the controller needs to be tuned once the structural decision regarding that particular loop is taken.

Role of Simulation Models: Simulation tools are very useful for tuning. Often, preliminary tuning of flow, level and pressure loops is a trivial task and can be done fairly easily based on standard guidelines (Luyben, 2002). But composition and temperature loops need careful tuning. Making use of built-in tools in dynamic simulators is effective; for example, auto-tuning (closed loop relay-feedback technique) can be used to estimate good initial controller settings. One of the advantages of auto-tuning is that it can also be used for open-loop unstable systems if there exists a stable limit cycle (Yu, 1999).

Level 3: Structural decisions regarding product specifications should be taken even before considering the process stability which is the basic criterion of any control system.

Production Rate Manipulator Selection: This involves identifying the primary process path (from main raw material to main product). Many primary process paths may exist when there are several raw materials and products. Each primary process path may be considered to develop alternatives if the best one cannot be found at this stage. After identification of the primary process path, internal/implicit variables on this path are preferred as the throughput manipulators (TPMs) over external/explicit variables (fixed-feed or on-demand) as the former are found to be dynamically more effective (Price and Georgakis, 1993). The former are usually associated with the reactor operating conditions. Between fixed-feed or on-demand options, the former is preferred over the latter as it is shown to be superior in terms of performance (Price and Georgakis, 1993; Luyben, 1999).

Role of Simulation Models: The dynamic simulation model cannot be made use of to take the decision about the TPM at this stage as the overall control strategy is not yet in place. But, as a good starting point, one can make use of steady-state simulation model to choose the primary process path. Some processes may have multiple inputs and outputs with several reactions taking place in the reactor, in which case this procedure will be of great use. For example, for processes involving dominant side reactions the most intuitive TPM (e.g., limiting reactant flow rate) may not be the best. After selecting the primary process path, the TPM can be selected along this line by using a steady-state simulation model. Obviously the one with maximum steady state gain will be the preliminary choice as the TPM.

Product Quality Manipulator Selection: In this step, one selects the manipulated variable (MV) for product quality. Other composition loops, if any, will be dealt with after the material inventory loops (levels) are taken care of as the latter respond faster and so better handles need to be reserved for levels. In addition, as most of the levels are integrating (non-self-regulating), level loops need to be given priority over composition loops as stability concerns are associated with levels. Hence, other composition loops will be dealt in level 5 (control of unit operations).

Role of Simulation Models: This stage deals with product purity, which is often a local decision; i.e., manipulator for product quality can be found in/around the unit with which the product stream is associated (Luyben, 1993). Though the product quality is a local decision, it has to be considered before other plant-wide decisions (such as material inventory and component balances) because of its ultimate importance. The unit producing the product stream can be separately simulated for selecting the best manipulator for product quality. Other structural decisions that are taken for simulating the unit need not be the best from the overall plant point of view and so these decisions need not be carried forward to the next levels except the product quality manipulator.

Level 4:

Selection of Manipulators for More Severe Controlled Variables: Process constraints such as equipment and operating constraints, safety concerns and process stability issues will be dealt with in this stage as they have severe operability implications.

Role of Simulation Models: Dynamic simulation model can be made use of to choose the best manipulators for meeting severe process constraints. Good initial estimates for the tuning parameters can also be obtained using in-built tools of the simulator such as auto tuning.

Selection of Manipulators for Less Severe Controlled Variables: Levels need to be taken care of while ensuring that the levels in the primary process path are self-consistent (Appendix A). Other levels that are not in the primary process path should be controlled in such a way that the control will direct the disturbances away from the primary process path. Last, pressures (often self-regulating in nature) need to be controlled.

Role of Simulation Models: Level loops are placed so that they will form a self-consistent structure. Process knowledge from simulation must also be used while taking the decisions based on heuristics. Decision supported by simulation must be chosen in the case of any conflict because heuristics need not always be true. Finally, pressure loops can be placed with the aid of dynamic simulation models. In highly integrated processes, with long gas-processing lines, it is often difficult to decide whether to control the pressure at a particular location or not. For example, in the TE process, it is often adequate to control the pressure of the vapor in an entire section of the process by using a manipulator at a single location and allowing the remaining vapor inventories to float, if the pressure drops in the gas loop are small. Dynamic simulation model would be of great use while taking this decision.

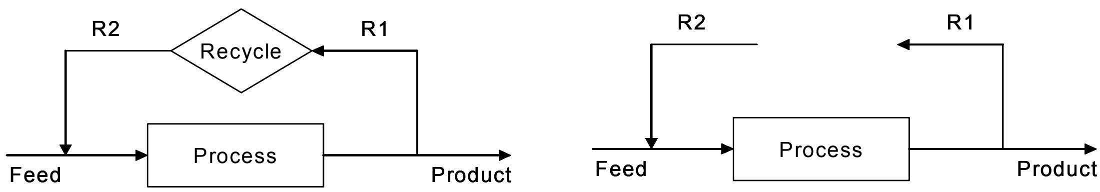
Level 5:

Control of Unit Operations: *Control of individual unit operations* is considered prior to *checking component material balances*. By doing so, some of the component inventory loops will be implicitly taken care of in this stage thereby making the analysis in the next stage (checking component inventory) easier.

Role of Simulation Models: At this level, all the individual unit operations can be simulated. This step mainly deals with the composition loops (or temperature loops) as all other loops (levels and pressures) have already been taken care of in the earlier stages. While placing the control loops on individual unit operations one must ensure that the plant-wide objectives are not violated (for example, one can simulate different disturbance scenarios with the primary units in the process to see if any of the aforementioned plant-wide objectives are violated). Finally, these can be tuned using the built-in tools of simulators.

Level 6:

Check Component Material Balances: Component inventory control can be assured in the case of single-unit operations, but from plant-wide perspective, component inventory may not always be self-regulating as it usually involves reaction and separation sections with recycles. This characteristic feature urges coordination of various control strategies over different sections in the plant to ensure that the rate of accumulation of each component in the overall process is zero. In addition, designing the control systems for highly integrated processes is really challenging because of recycles. To develop efficient control systems, the designer needs to understand the severity of the recycles. To do so, it is proposed to compare the plant behavior with and without recycle loop (as illustrated in Figure 3.1) in Level 7. Hence, in the present step, analysis is carried out without recycle loop and effect of recycles is considered in the next level. This approach is essential for isolating the problems that may arise due to component inventory regulation and recycles, thereby making the overall problem more easily tractable.



(a) **(b)**

Figure 3.1: Schematic showing (a) Process with Recycle and (b) Process without Recycle (obtained by removing recycle block, i.e., tearing the recycle loop). Streams R1 and R2 will still have base case steady-state values. Removal of the recycle stream (R2) is not desirable as the process will then have entirely different behavior‡.

‡ At times, the process without recycle stream (i.e., R2) may be more economical. In that case, process design can be modified (by removing the recycle stream) and control system can be designed. However, the focus in this chapter is to design the control system for a given process and process design modifications are not considered. Such design modifications are considered in the 'integrated design and control' study that is carried out in Chapter 6.

Role of Simulation Models: In simulation, flow rates of all components at various locations can be accessed. Using these along with reaction stoichiometry to account for generation and consumption of components via reactions, accumulation tables can be prepared to check whether the rate of accumulation is zero while the plant without recycle loops is in operation (i.e., while the simulation is running). If there is any accumulation, process topology must be analyzed carefully to ensure that some component inventory loops are not forgotten. In some complex processes, it is difficult to ensure that all the inventory loops are in place. So, one can make use of simulation to ensure that all the inventory loops are placed according to the process requirements.

Level 7:

Effects due to Integration: This step needs to be analyzed only after all the above issues (in the previous steps) have been taken care of. Luyben et al. (1999) considered this step in the earlier stages. Their reasoning is that the plant-wide decisions need to be given higher priority and therefore need to be satisfied in the earlier stages. But the hierarchy should ideally be based on how severe the integration effects are from a plant-wide perspective. One can argue that, if found to be very severe based on the steady-state analysis, this step can be done earlier and Luyben's rule can be applied. However, in this case, the probability of arriving at unbalanced structures and self-inconsistent structures would be higher, which is not desirable. Besides, from our tests with simulators, it is observed that there is an inherent interlink between component inventory regulation and introduction of recycles. It would thus be easier and more appropriate to analyze them in consecutive steps. Hence, it is better to analyze the integration effects at the end and take appropriate action. There are no solid guidelines at this stage except making use of rigorous simulation models to design a workable control strategy. It would give the control engineer flexibility to choose the better one which otherwise would have been eliminated by applying some heuristics. Note that Luyben's rule is not rejected here but considered as one of the potential alternatives based on necessity, rather than as a rule.

Role of Simulation Models: To understand the severity of the recycle dynamics, the process with and without the recycles should be simulated for anticipated disturbances[§]. Typically, the process with the recycles exhibits slower (or even unstable) dynamics. If not, the recycle dynamics can be concluded as not severe. In the case of slower or unstable dynamics, the control structure has to be altered either by including additional control loops or by revising the control decisions that have been taken in the earlier stages. Decision making at this stage is going to be process-specific and hence cannot be generalized. One can try out the two suggestions in the improved heuristic methodology (Table 3.1). These guidelines need not necessarily result in a control system with satisfactory performance and stability requirements. In such a case, rigorous simulation can be used to troubleshoot the process. Needless to say, the decisions in the earlier stages need to be revised, if a workable control strategy cannot be generated at this stage. Finally, one can simulate and evaluate the performance of alternative control structures, if any, to find the best.

Level 8:

Enhance Control System Performance, if possible: The designer can look into possible modifications to further enhance the performance of the control system. For example, one can look into re-configuring the loops or re-structuring the control

[§] Since there can be several recycles, this analysis can be carried out sequentially (i.e., one disturbance at a time) to gauge the impact of respective recycle on the overall process dynamics. Throughput changes (with different magnitudes) should be considered in this analysis since they are not only the most common type of disturbances but they also severaly affect the overall process dynamics.

system. One can even analyze the necessity and feasibility of implementing advanced control strategies.

Table 3.1: Improved Heuristic Methodology

Level	Things that need to be dealt with
1	1.1. Define PWC Objectives
	1.2. Determine CDOF
2	2.1. Identify and Analyze Plant-Wide Disturbances
	2.2. Set Performance and Tuning Criteria
3	**Product Specifications**
	3.1. Production Rate Manipulator Selection ➢ Identify Primary Process Path ✓ Implicit/Internal Manipulators ✓ Explicit/External Manipulators • Fixed Feed Flow Control • On-Demand Control
	3.2. Product Quality Manipulator Selection
4	**“Must-Controlled” Variables**
	4.1. Selection of Manipulators for More Severe Controlled Variables ➢ Process constraints (equipment and operating constraints, safety concerns, environmental regulations) especially those associated with reactor
	4.2. Selection of Manipulators for Less Severe Controlled Variables ➢ Material Inventory – Levels for Liquid & Pressures for Gases ✓ Levels in Primary Process Path – Make sure the control will be self-consistent ✓ Levels in Side Chains – Make sure that the control structure will direct the disturbances away from the primary process path ✓ Pressures in the process
5	**Control of Unit Operations**
6	**Check Component Material Balances**
7	**Effects Due to Integration (i.e., Due to Recycles)**
	Identify Presence of Snow Ball Effect and Analyze it’s Severity ➢ Analyze the need to fix composition in the recycle loop to arrive at a balanced control structure ➢ Or, is it necessary to fix a flow at a strategic position in the recycle loop?
8	**Enhance Control System Performance, if possible.**

The proposed integrated framework is clearly more detailed on how to go about the PWC problem and can be applied to any industrial process. The framework is logically developed and has several new features as indicated below:

- Heuristics-based methodology is improved with more specific and useful guidelines wherever necessary.
- The sequence in Luyben's heuristics-based methodology is altered to facilitate the use of rigorous nonlinear simulation models and also to make the PWC problem more tractable. For example, severity of the recycle dynamics is systematically analyzed, to take necessary corrective action, towards the end (i.e., in the 7th stage).
- Several studies in the past used dynamic simulation to validate and evaluate alternative control system designs after they are developed. On the other hand, the proposed framework integrates heuristics and simulation models at each stage of the procedure (and not simply at the end) to achieve greater insight. This has several benefits.
    - The rigorous simulation models are very useful in gauging and screening any of the heuristics thereby resulting in more efficient control system(s).
    - The proposed framework is likely to reduce the number of alternative control systems (by screening un-attractive alternatives at each stage) that need to be evaluated at the end thereby making the overall task easier.
    - The integrated framework will be very useful to novices as simulation models offer virtual hands-on experience, while the heuristics serve as guidelines to design effective control systems.
    - The framework will increase applications of dynamic simulation of process plants, which is often not possible without a basic regulatory control system.

3.3 Overview and Simulation of the HDA Process

The most widely utilized test-beds for the PWC studies are the TE plant (Downs, 1993) and the classical reactor-separator-recycle section. These have been proved to be beneficial for the PWC community to better understand the PWC problems. However, there is a need to study additional processes which are of practical importance (i.e., typical industrial processes with real components and many standard unit operations) and complex enough (with material and energy recycles) to be representative in its essential features as PWC applications. So, we have chosen the HDA process which is a highly integrated and nonlinear petrochemical process. The presence of heat integrated adiabatic plug flow reactor (PFR) with exothermic reactions and three multi-component, high purity distillation columns and high level of interaction (because of the presence of material and energy recycles) makes it really a challenging process for control system design. Some reported studies on the HDA process are by Luyben et al. (1999) and Qiu et al. (2003).

3.3.1 HDA Process Description

In the HDA process, fresh toluene (pure) and hydrogen (H_2) – i.e., 95% H_2 and 5% methane, (CH_4) - are mixed with recycled toluene and H_2 (Figure 3.2). This reactant mixture is preheated in a feed-effluent heat exchanger (FEHE) using the reactor effluent stream and then heated to the reaction temperature in a furnace before being fed to the adiabatic PFR. Two main reactions taking place inside this reactor are:

Toluene + H_2 → Benzene + CH_4

2 Benzene ↔ Diphenyl + H_2

The reactor effluent is quenched with a portion of the recycle separator liquid to prevent coking, and further cooled in the FEHE and cooler before being fed to the flash separator. A portion of unconverted H_2 and CH_4 overhead vapor from the separator is purged (to avoid accumulation of CH_4 within the process) while the remainder is compressed and recycled to the reactor. The liquid from the separator is processed in the separation section consisting of three distillation columns. The stabilizer column removes H_2 and CH_4 as the overhead product, and benzene is the desired product from the product column top. Finally, in the recycle column, toluene is separated from diphenyl, as the distillate and recycled back.

3.3.2 Steady-State Simulation

The success of any steady-state simulation model largely depends on the selection of a suitable thermodynamic package (Carlson, 1996; Horwitz and Nocera, 1996; Benyahia, 2000). In this study, the improved Peng-Robinson (PR) equation of state is selected for property estimation as it is very reliable for predicting the properties of hydrocarbon-based components over a wide range of conditions and is generally recommended for oil, gas and petrochemical applications. With the use of default templates in HYSYS, the steady-state simulation model of the HDA process has been developed according to the flow-sheet topology (Figure 3.2) and the process information from Douglas (1988). Though Douglas (1988) considered 75% as the optimal conversion, recent studies by Phimister et al. (1999) showed that the optimal conversion is 70% and hence the base case HDA process flowsheet is developed based on 70% conversion. This variation is not unexpected and can be qualitatively explained based on the variation in the feedstock and utility prices since 1988.

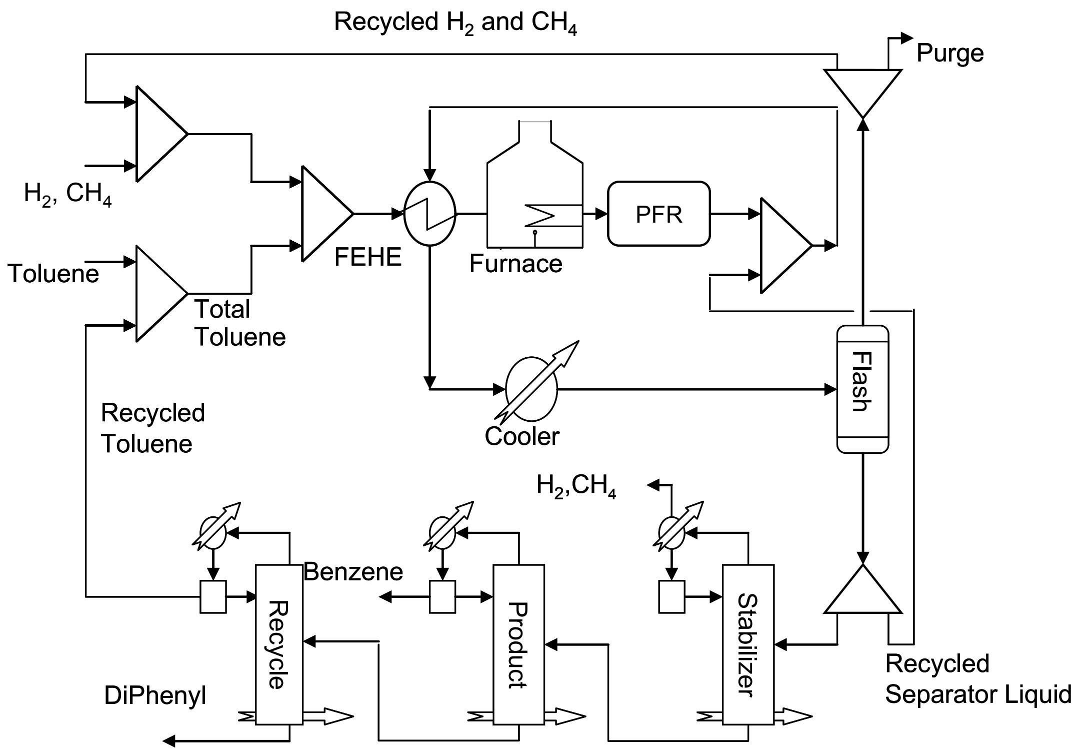


Figure 3.2: HDA Process Flow-Sheet to Produce Benzene from Toluene

Distillation columns are modeled by rigorous tray-by-tray calculations. Preliminary estimates of the number of trays and feed tray location have been calculated using the shortcut methods. Rigorous modeling is extremely important especially while designing the equipment such as distillation columns which has a great impact on control studies. For example, Douglas (1988) assumed constant vapor flow rate in the stabilizer for sizing, which is satisfactory for preliminary design. The steady-state simulation of the stabilizer shows that there is significant variation in vapor flow rate from top to bottom. Hence, the assumption of constant vapor flow rate in the stabilizer is not valid and inappropriate for control studies.

A point worth noting while building steady-state simulation models for complex industrial processes (with many recycles), such as the HDA process, is the inadequacy of the default tolerance limits of recycle blocks. It is observed that these default tolerance limits fail to give reasonably accurate results. This causes accumulation in the process which in turn makes the initial transients longer in dynamic simulation as we can use the same steady-state model in dynamic mode also with some modifications. So, we need to pay considerable attention to the recycle tolerances to get reasonably accurate results. Not only the recycle tolerance limits, but the number of recycles and the location of recycle blocks also affect the computational efficiency. Thus, in general, recycles pose convergence difficulties while developing steady-state simulation models (e.g., Schad, 1994 and 1998). However, such problems can be resolved by making use of “recycle assistant”, which is an added feature in the newer versions of HYSYS (i.e., Aspen HYSYS 2004 or later versions). Recycle assistant aids the user to place the recycles in strategic locations in such a way that the number of recycles can be minimized, and thus the convergence can be achieved in less number of iterations.

3.3.3 Moving from Steady-State to Dynamic Simulation

HYSYS provides an integrated steady-state and dynamic simulation capability. In this integrated simulation environment, the dynamic model shares the same physical property packages and flow-sheet topology as the steady-state model. Thus, it is easy to switch from steady-state to dynamic mode. However, there are several differences in both these environments in terms of specifications and solution methodology. One major difference is the pressure drop in distillation columns; a constant value has to be specified for this in steady-state mode whereas it will be calculated in dynamic mode based on the given tray data. So, while moving to the dynamic mode, a systematic procedure of many steps, namely, plumbing, Pressure-Flow (P-F) specifications and equipment sizing, needs to be followed, which are briefly discussed below (Luyben, 2002).

Plumbing: To take care of some of the dynamic effects introduced in the dynamic mode, the flow-sheet topology may have to be modified by placing the additional units such as pumps wherever necessary and this is called plumbing. One of the important steps in plumbing is placement and sizing of the control valves in the process. For realistic dynamic simulations, the "plumbing" in the flow-sheet should be appropriately done to ensure the flow of material from one unit to another.

P-F specifications: In dynamic mode, we need to give additional specifications besides the usual steady-state specifications (for material and energy balance calculations). These additional specifications are known as P-F specifications. The numerical integration technique that is used to solve the resulting equations in dynamic mode is implicit Euler method with fixed step-size. Usually pressure specifications are preferred over flow specifications as the "pressure-driven" mode of simulation is more realistic, especially for the processes in which the hydraulics and fluid mechanics are of vital importance. However, in some cases flow specifications need to be given.

Equipment Sizing: As the dynamics of any unit is dependent on size of the equipment, various units (e.g., distillation columns) need to be sized before moving to dynamic mode which can be done using in-built tools such as tray sizing utility.

In principle, we can then switch over to dynamic mode at this stage. However, considering the complex nature of the highly integrated processes with several recycles, open-loop dynamic simulation of the entire process may not be possible and/or useful for analysis due to the overlapping effects of many phenomena. Thus, it is advisable to place at least some key loops before running any plant-wide dynamic simulations. For example, if there is any problem while simulating, it is difficult to identify whether the problem is due to improper specification(s) or inefficiency of the control system. So, proper guidelines are necessary at this stage to resolve this problem. This is where heuristics can aid us to proceed further via a step by step systematic procedure. Both the steady-state and dynamic simulation models are made use of to integrate simulation with the proposed improved heuristic methodology to design the PWC system for the HDA process in the following section. It should be noted that all the dynamic simulations in this and also in the subsequent chapters are carried out without any noise.

3.4 Application of Proposed Methodology to the HDA Process

The dynamic simulation model of the HDA process consists of 959 nonlinear, highly coupled algebraic and differential equations. This part of the study would also reveal the capability of dynamic simulation in the context of PWC.

Step 1.1: Define PWC Objectives

1. Production Rate - 280 lb mol of benzene/hour (9.92 tonnes/hour)
2. Product Quality - Benzene purity ≥ 99.97%
3. Process Stability - The feed effluent heat exchanger with plug flow reactor has been simulated and perturbed with and without heat integration, and the results reveal that the process with heat integration is operating at unstable steady-state. It has also been observed that maintaining the reactor inlet temperature at a constant value stabilizes the process.
4. Process Constraints (Douglas, 1988):
   - The temperature at the reactor inlet should be around 1150 ^{o}F. This is an optimization decision to have better reaction rates.
   - The ratio of H_2 to aromatics (i.e., benzene, toluene, and biphenyl) has to be at least 5 at the inlet. This is basically to provide a thermal sink to avoid

coking that takes place at higher temperatures. Also, excess H_2 encourages the primary reaction and discourages the secondary reaction (Smith, 1995).

- The temperature at the reactor outlet should not exceed 1300 ^oF to avoid coking.
- The outlet stream from the reactor must be quenched to 1150 ^oF to prevent thermal decomposition of products and to avoid fouling in FEHE.

Step 1.2: Determine CDOF

Available CDOF is found to be 23 (Luyben, 1999).

Step 2.1: Identify and Analyze the Plant-Wide Disturbances

The important plant-wide disturbances in the HDA process are ± 25% variation in toluene feed rate, - 2.5% variation in H_2 feed purity and ± 5% variation in the set-point of flash drum level. From the steady-state simulation model, it is observed that 5% variation in the toluene feed flow rate produced a large variation, up to 20% in the flows of separation section; and, 85% variation is observed in the separation section flows for 25% variation in the toluene feed flow rate. This information will be useful while taking tuning decisions in the next step.

Step 2.2: Set Performance and Tuning Criteria

Settling time is chosen as the performance criterion for the preliminary studies. The analysis in the previous step showed that small variations in the toluene feed flow rate produced larger variations in the flows of separation section. So, separation section controllers must be more conservatively tuned compared to those in other parts of the plant.

Step 3.1: Production Rate Manipulator Selection

From steady-state simulation, the steady-state gain of toluene to benzene is found to be much larger than that of H_2 to benzene. So, the primary process path can be selected as toluene to benzene (Figure 3.2). As reactor conversion is an optimization decision, reactor conditions (internal TPMs) like temperature etc., cannot be used as the TPMs. So, the next best alternative i.e., fixed-feed flow of toluene, is considered as the TPM. Jorgensen and Jorgensen (2000) reported that the H_2 feed stream is the better TPM than the toluene feed stream. Their contention is that the toluene as the TPM fails to account for the side reaction and increasing the H_2 concentration limits the extent of side reaction leading to better selectivity and higher production rate. At first sight, Jorgensen and Jorgensen's (2000) argument seems to be alright. However, it fails to take into consideration the extent of reactions. From the steady-state simulation, it can be seen that the extent of side reaction is negligible when compared to that of the main reaction. In this regard, toluene would still be a better TPM because of its larger gain.

Step 3.2: Product Quality Manipulator Selection

Based on RGA analysis (Svrcek et al., 2000) of the benzene column, it is found that both the reflux flow and the distillate flow are equally good for controlling the composition of benzene in the product stream. Hence, the conventional structure with reflux as the manipulator for product quality is selected.

Step 4.1: Selection of Manipulators for More Severe Controlled Variables

The reactor inlet temperature is controlled by furnace duty and the PFR with FEHE is observed to be stable in the dynamic mode. Here the decision is quite straightforward. But in certain cases (e.g., if we consider bypass to FEHE) dynamic simulation can be used to make the decision. The initial estimates for the tuning parameters are calculated using the auto-tuning tool in HYSYS Dynamics. The second process constraint is on the H_2-to-aromatics ratio at the reactor inlet. So, H_2 feed is selected to maintain the ratio of H_2 to aromatics into the rector. In this case, it turns out to be a quite straightforward decision. It is implemented as a ratio control using spreadsheet available in HYSYS Dynamics. In the control strategy of Luyben et al. (1999), there is no explicit control of H_2 to aromatics ratio. However, it is advisable to handle the process constraints explicitly as in our case. The H_2-to-toluene ratio has been considered in the previous studies whereas the actual process constraint is on the ratio of H_2 to aromatics (McKetta, 1977). This constraint is very important as there can be coking if the H_2 to aromatics ratio is less than five and the process will not be economically attractive if the ratio is more than five. So, it is most advisable to have an explicit control over this process constraint.

The third process constraint is to maintain the outlet temperature of the reactor within 1300 ^{0}F. From the steady-state simulation model, it can be seen that the reactor outlet temperature (1220.1 ^{0}F) is well below 1300 ^{0}F. So, this is an inactive process constraint (even in the presence of worst-case disturbance) and an explicit control action is not needed. The last process constraint is to quench the reactor effluent stream to 1150 ^{0}F. From the process knowledge, the most intuitive manipulator is the quench stream from the flash drum.

Step 4.2: Selection of Manipulators for Less Severe Controlled Variables

Levels in the primary process path are controlled in the direction of flow (as fixed feed flow is the TPM) to have self-consistent structure (Appendix A and Figure A.1). But there is one unavoidable exception to this; the toluene column condenser level should not be controlled by distillate stream as it back-propagates the disturbances to primary process path. But the other immediate alternative, reflux flow as the manipulator, is very inadequate as the reflux ratio is very small (L/D = 0.05). This compelled us to violate the heuristic. Levels that are in side paths are controlled in such a way that the disturbances are directed away from the primary process path. Again, there is an exception here; according to this guideline, the toluene column reboiler level must be controlled by bottoms flow. Fonyo (1994) also considered bottoms flow as the manipulator for toluene column reboiler level which appears to be quite obvious. But dynamic simulations showed that the reboiler duty affects the reboiler level more than the bottoms flows and hence is a better MV for reboiler level control in the toluene column. This can be intuitively explained based on the fact that the reboil (boil-up) ratio is very high (~ 24) and bottoms flow rate (i.e., biphenyl) is very small (as the selectivity losses towards biphenyl for the base case HDA process are considerably low). These two examples show that the heuristics cannot always be relied upon. The heuristics simplify the overall task but they need to be applied with a good dose of engineering judgment and process-specific knowledge.

Finally, operating pressures of three distillation columns, and flash drum pressure are controlled appropriately. One interesting issue is the decision regarding pressure control in the gas line. When the process, such as the HDA process, has a very long gas line with many unit operations, it is difficult to decide the number of points at which the pressure needs to be controlled and their strategic locations. In this case, dynamic simulation can be used. For the HDA process, dynamic simulation showed that controlling the pressure in the flash drum would ensure the pressure control in the total gas line. Reactor pressure does not require any explicit control action.

Step 5: Control of Individual Unit Operations

In this step, all unit operations are analyzed and control loops are placed wherever necessary. Dual composition control for all the three distillation columns is considered as it is relatively more optimal than the single end composition control and also offers better control from the plant-wide perspective. For example, for the recycle column as an individual unit-operation, single end composition control should be sufficient as the main objective is not to lose toluene from the bottom stream. However, from a plant-wide perspective minimizing the disturbance propagation through the recycle stream is also as important as minimizing the toluene loss which results in dual-composition control. Hence, plant-wide perception is given due importance and dual-composition control is chosen for the recycle column.

Flash drum inlet temperature has to be controlled which can be achieved by the duty of the cooler before the flash. In some cases, there exists a strong correlation between temperature and pressure of an adiabatic flash. In these cases, either the temperature or the pressure can only be controlled. In the HDA case, the correlation is not strong and it is preferable to control both for better performance. So, flash temperature is also controlled.

Step 6: Check Component Balances

All the individual unit operations in the process are simulated separately and, from the component inventory tables, it is observed that the inventory of all components in all the units is regulated. However, there is no guarantee that the component inventory will be regulated when all the units are put together as there can be incompatibility among the control actions of different controllers. Hence, all the units are put together according to process topology (without gas and liquid recycles) and component inventory is observed to be regulated.

Step 7: Effects due to Integration

So far, the analysis is carried out without gas and liquid recycles (i.e., by tearing both the gas and liquid recycle streams as in Figure 3.1). All the control decisions that have been taken so far lead to a control system which is stable even with both the recycles. This control system is same as the one developed by Ponton and Laing (1993). Though they have qualitatively discussed the superiority of their control system over the control system designed by Stephanopoulos (1984), they did not report any simulation results to show the performance of their control system. Moreover, there is no additional consideration for recycles in the analysis of Ponton and Laing (1993). As shown in the following analysis, a better control system is generated by systematically analyzing the effect of recycles on overall plant dynamics.

Effect of Gas Recycle on Overall Plant Dynamics: The closed-loop dynamic simulation is run with each of the expected disturbances for the HDA process with and without gas recycle, and the effect of gas recycle on the overall plant dynamics is observed to be negligible when compared to that of liquid recycle (discussed in the following section). Possible reasons for this are as follows: (1) gas recycle dynamics are usually faster than liquid recycle dynamics; (2) any variation in the gas recycle can easily be attenuated by the H_2/aromatics ratio controller; (3) the liquid recycle dynamics in the HDA process (Figure 3.2), are more complex compared to the gas recycle dynamics because of the presence of three distillation columns with nonlinear dynamics. Hence, further analysis is carried out based solely on the impact of liquid recycle dynamics on the overall dynamics. This can further be justified based on an analogy from reaction engineering: the slowest of all (parallel) reactions is the rate limiting step and the analysis can be carried out by ignoring faster reactions.

The gas recycle also contains a purge stream to avoid accumulation of CH_4 in the process and, hence, a composition controller (CC) is needed to make the CH_4 inventory in the process self-regulating. The composition of the purge stream is controlled by manipulating recycle gas flow as it is the larger of the two potential manipulators available - gas recycle and purge flows. So, composition loop is placed by making use of the compressor duty as the manipulator, which in turn manipulates the gas recycle flow rate. This strategy is equivalent to manipulating steam flow rate to control gas flow rate in the case of a steam turbine driven centrifugal compressor. This strategy is the most energy-efficient (Luyben, 2002) and hence implemented in our study. Alternatively, gas recycle stream can be manipulated by compressor suction throttling (or bypassing) or purge flow rate manipulation which in turn affects the gas recycle flow rate to control purge composition.

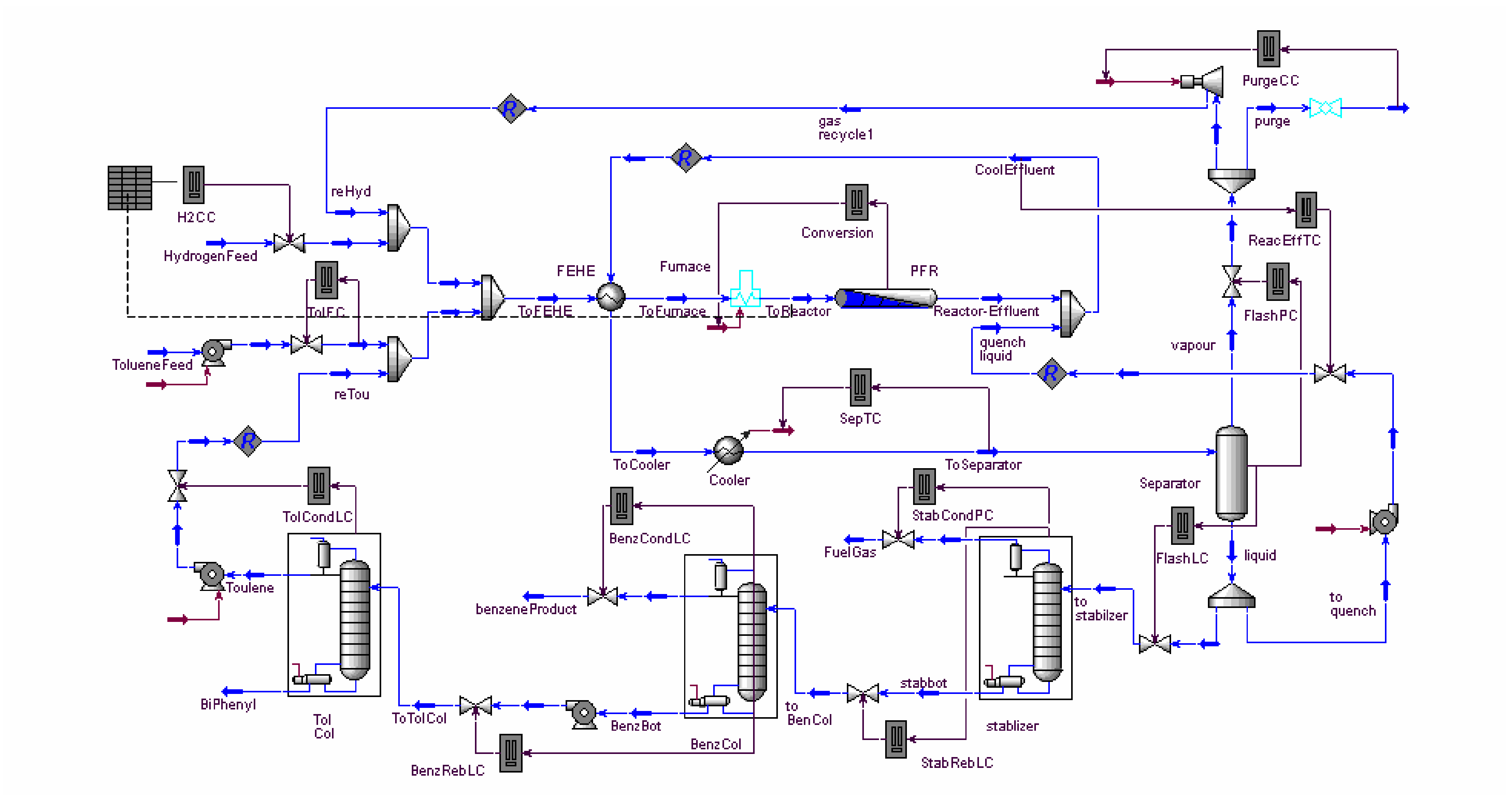
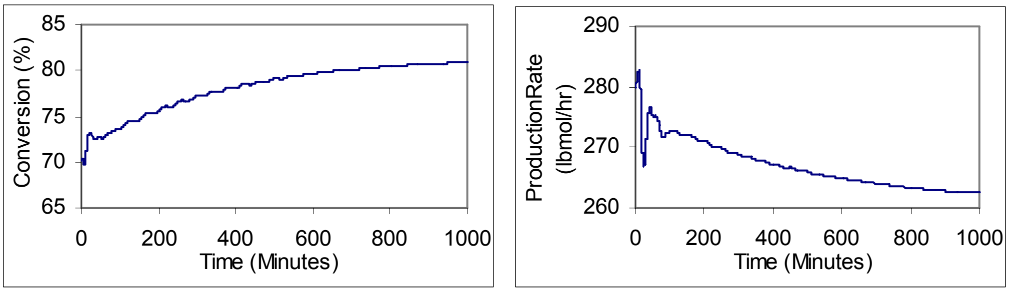


Figure 3.3: Dynamic Simulation Model of the HDA Process showing the Controllers Designed by the Proposed Methodology

Effect of Liquid Recycle on Overall Plant Dynamics:

Problem Identification: Both the gas and liquid recycles are closed and the closed-loop dynamic simulation is run for 5% and 25% variation in the toluene feed flow rate. Though the closed-loop system is stable, three main inefficient features of the control system in handling the disturbances are observed.

1. The control system is able to settle the process at some steady-state but, as can be seen from Figure 3.4a, the conversion at the new steady-state (~ 80%) is different from the optimal conversion (~ 70%).



(a) **(b)**

Figure 3.4: (a) Conversion and (b) Production Rate Transients for the Process (with Recycles and before Installing Conversion Controller) for 5% Variation in Toluene Feed Flow Rate

2. Although the control system is able to attenuate the 5% load disturbance, it is taking too long (around 1000 minutes) to reach the new steady-state (Figure 3.4). Qualitative analysis to this poor performance can be given - conversion is a typical kind of process variable, particularly for the HDA process, which affects almost all other process variables because of the highly integrated nature of the process. So, unless the conversion settles, it is not possible for any other controller in the process to settle down. Hence, it is advisable to keep the conversion constant for better performance of the control system.
3. For the worst-case disturbance of 25% variation in toluene feed flow rate, some liquid level control loops, especially those in the recycle loop, are hitting the equipment/valve constraints; Figure 3.5 shows actuator saturation in the control

loop for level in the recycle column condenser, which is not desirable. It is advisable to operate a valve between 10 and 80% of the valve stroke across the expected range of operation (Bishop et al., 2002).

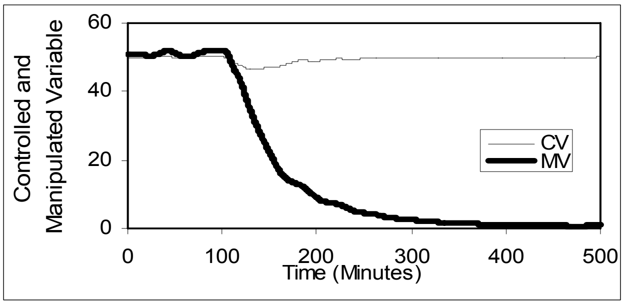


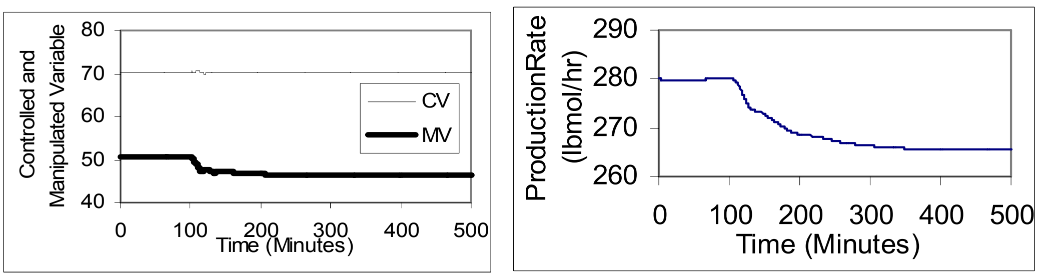
Figure 3.5: Recycle Column Condenser Level Response to 25% Increase in Toluene Feed Flow Rate in the Process with Recycles and before Installing Conversion Controller

Root Cause Analysis: It is suspected that the liquid recycle is the root cause because everything else has been taken care of systematically in the earlier stages. To confirm this, the process without liquid recycle is simulated for the same disturbance (5% variation in the toluene feed flow rate). Now the process is able to handle the disturbance and quickly reaches new steady-state which is not far away from the optimal steady-state (unlike the process with liquid recycle). Hence, it can be concluded that the liquid recycle is creating additional problems which need to be taken care of.

Identifying the Solution: Based on the analysis given in the *Problem Identification* section above, controlling the conversion (or reactor outlet toluene concentration) is one of the promising alternatives.

Choice of manipulator for conversion controller: There can be basically three potential manipulators: 1) reactor inlet composition, 2) pressure and 3) temperature. However, there are additional constraints (both economical and operational) on inlet composition (i.e., ratio of H_2 and aromatics) and cannot be considered as a manipulator for conversion. Of the remaining two alternatives, temperature is found to be more dominating. Hence, reactor inlet temperature is selected as the manipulator (which in turn was manipulated by furnace duty).

The closed loop simulation, carried out (for expected disturbances) with conversion controller, is found to overcome all the above-mentioned problems: (1) Figure 3.6a shows that the conversion has been controlled at the optimal value (~ 70%) despite the presence of the disturbance. (2) As the conversion settles very fast (Figure 3.6a), other process variables also settle down quickly; Figure 3.6b shows that production rate just took around 200 min to reach steady-state. (3) The control system is able to handle the worst-case disturbance without hitting the equipment constraints; Figure 3.7 shows the response of the toluene column condenser level controller (LC). Thus, the conversion controller provides a balanced control structure by distributing the effect of load disturbance to different points in the plant, say, reaction and separation sections. Hence, it is essential to have the conversion controller. Except Ng and Stephanopoulos (1996) and Douglas (1981) nobody else has made use of conversion controller for the HDA process. However, they did not give any simulation results for the use of conversion controller.



(a) (b)

Figure 3.6: (a) Conversion (b) Production Rate Transients for the Process with Liquid Recycle after Installing Conversion Controller for 5% Variation in the Toluene Feed Flow Rate

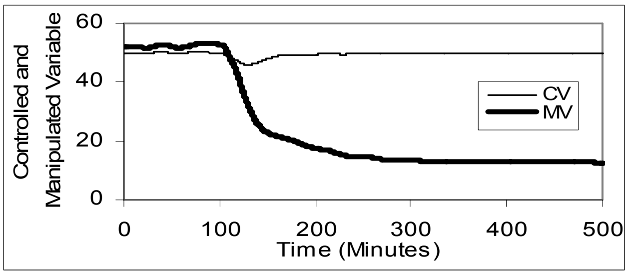


Figure 3.7: Recycle Column Condenser Level Response to 25% Variation in Toluene Feed Flow Rate for the Process with Liquid Recycle and Conversion Controller

Justification for the introduction of conversion controller: It is observed (from Table 3.2) that introduction of the conversion controller does not make much difference when there is no liquid recycle. So, there is no need for conversion controller for the process without liquid recycle. However, for the process with recycle, the conversion controller gives superior performance (Figure 3.8). Hence, the conversion controller is required as introduction of liquid recycle is causing the control system to take longer time to regulate the component inventories because of the recycle dynamics. From Figure 3.8, it can be observed that the conversion controller suppressed the recycle effects and consequently, the control system performance is closer to what could have been achieved if there were no recycles. Thus, the conversion controller here conceptually resembles the "recycle compensator" used by Scali and Ferrari (1999). Further justification for the conversion controller can be given based on the steady-state implications. From the steady-state simulation model, the snowball effect is found to be more severe (85% variation in the recycle flow rate for 25% variation in the feed flow rate) in the case of constant temperature controller (TC) than that (25% variation in the recycle flow rate for 25% variation in the feed flow rate) in the case of constant conversion controller. Dynamic simulations also confirmed this observation.

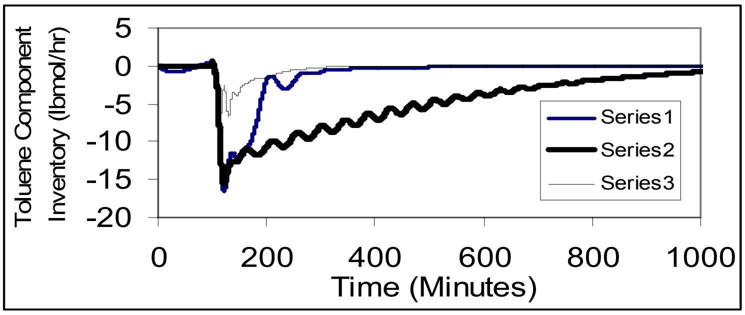


Figure 3.8: Toluene Inventory Transient for 5% Variation in Toluene Feed Flow Rate.
Series 1 - Without recycle and before installing conversion controller;
Series 2 - With recycle and before installing conversion controller;
and Series 3 - With recycle after installing conversion controller.

Control system performance under different situations – with and without recycle, and with and without conversion controller, is summarized in Table 3.2, which indicates an interrelationship among the recycle component (toluene) inventory, introduction of the recycle and performance of the control system. Hence, it is appropriate and easier to study the '*check component balances'* and '*effects due to integration'* in consecutive steps. Also, the summary in Table 3.2 emphasizes the importance and usefulness of dynamic simulation in order to design efficient control systems.

Table 3.2: Effect of Recycle on Component Inventory Regulation and Control System Performance

	Without Liquid Recycle		With Liquid Recycle	
	Without Conversion Controller	*With Conversion Controller*	*Without Conversion Controller*	*With Conversion Controller*
Conversion (*Measure of Economic Performance)*	72% (√)	70% (√)	80% (×)	70% (√)
Settling Time (*Measure of Dynamic Performance)*	200 (√)	100 (√)	1000 (×)	200 (√)
Equipment Constraints (*Measure of Safe Operation)*	√	√	×	√

Note: × - not desirable and √ - good/acceptable

3.5 Evaluation of the Control System

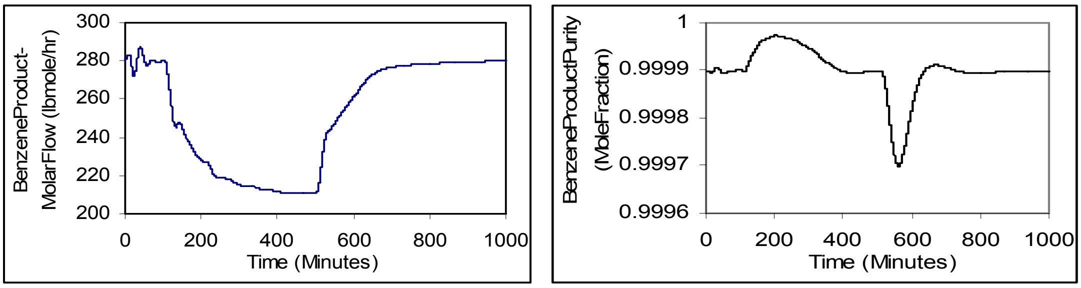
The control system designed for the HDA process has 23 control loops (Figure 3.3). The complete plant with this control system but without any disturbance is simulated for 100 mins. The set point, process variable and controller output of all the control loops are reported in Table 3.3, which shows that all the process variables are maintained close to their set-points. In the absence of the disturbances, we usually expect the controller output near 50% valve opening as they are designed for 50% opening at steady-state base case conditions. However, this is not so for some loops in Table 3.3 because pressures at different nodes in the dynamic mode are calculated by pressure-flow solver whereas they are specified in steady-state mode. This leads to some pressure variations within the process in the dynamic mode when compared to the steady-state mode. So, there is small offset from 50% in some of the valve openings as they depend on the neighboring pressures also. The LC in the flash drum (No. 1, FlashLC controller in Table 3.3) has settled at 68.71% opening because of liquid choking (flashing) inside the valve.

Various disturbances (load and set-point variations) are now introduced, and the transient responses of some important process variables are given in Figures 3.9 to 3.13 to show the effectiveness of the control system. It can be seen that the control system is able to attenuate the disturbances in reasonable settling time, which varies depending on the nature of the loop (Figures. 3.9 to 3.13).

Table 3.3: Values of Set Point (SP), Process Variable (PV) and Controller Output (OP) of all Controllers after 100 min of Simulation Time

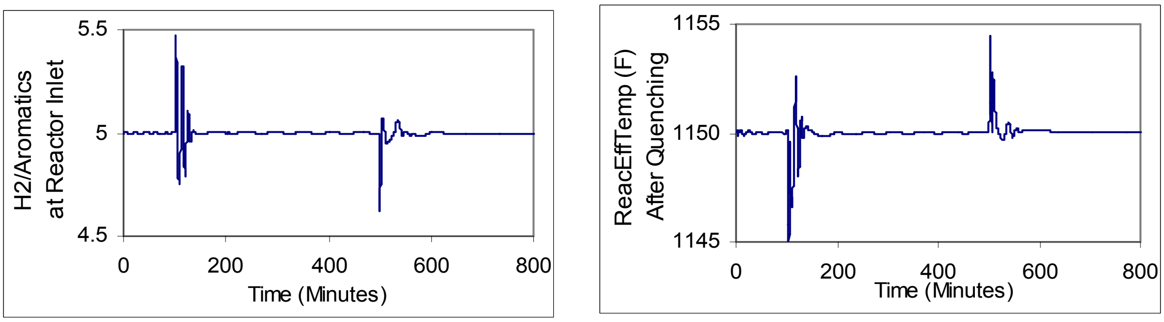
No.	Controller	SP	Process Variable	Controller Output
1	Flash LC	50.00	51.87	68.71
2	StabRebLC	50.00	50.09	50.18
3	StabCondLC	50.00	50.81	45.96
4	StabCondPC	9.826	9.824	51.26
5	BenzCondLC	50.00	49.82	49.63
6	BenzRebLC	50.00	49.88	49.76
7	BenzCondPC	2.246	2.247	50.10
8	TolCondLC	50.00	49.02	48.04
9	TolRebLC	50.00	50.17	50.87
10	TolCondPC	2.177	2.169	49.41
11	FlashPC	31.98	31.98	49.35
12	TolFC	290.0	290.0	51.55
13	H2CC	5.000	5.000	51.08
14	PurgeCC	0.6013	0.6013	52.15
15	BiPhenylCC	0.9999	1.0000	52.89
16	StabCC	112.2	112.2	49.75
17	BenzCC	130.5	130.5	50.33
18	Conversion	70.12	70.12	50.54
19	MCC (MethaneCC)	0.9129	0.9129	49.24
20	BCC (BenzeneCC)	0.9999	0.9999	50.39
21	TCC (TolueneCC)	0.9999	0.9999	53.73
22	ReacEffTC	621.1	621.1	50.70
23	SepTC	37.78	37.78	50.00

Feed Flow Rate Disturbance: At 100 min, -25% variation in the feed toluene supply rate is introduced as the disturbance and later removed at 500 min. In both the cases, the control system is able to attenuate the disturbances (Figures. 3.9 to 3.11). The transient in the first 100 minutes is due to switching from steady state to dynamic mode.



(a) (b)

Figure 3.9: (a) Production Rate (b) Product Quality Transients due to Load Disturbances in Toluene Feed Flow Rate



(a) (b)

Figure 3.10: (a) Hydrogen to Aromatics Ratio (b) Reactor Effluent Temperature (after Quenching) Transients due to the Load Disturbances in Toluene Feed Flow Rate

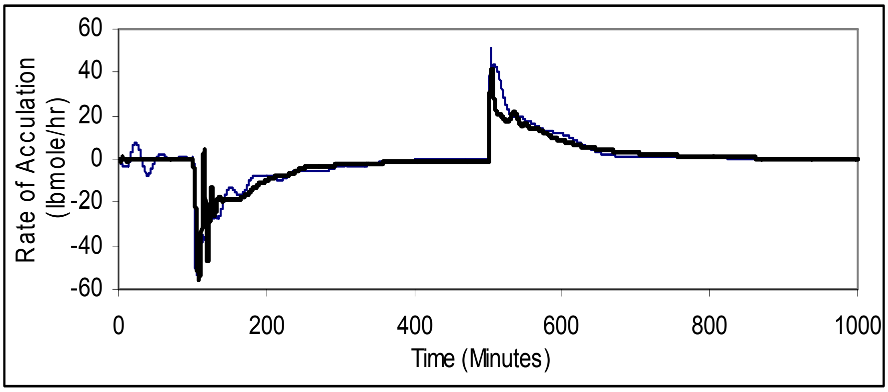
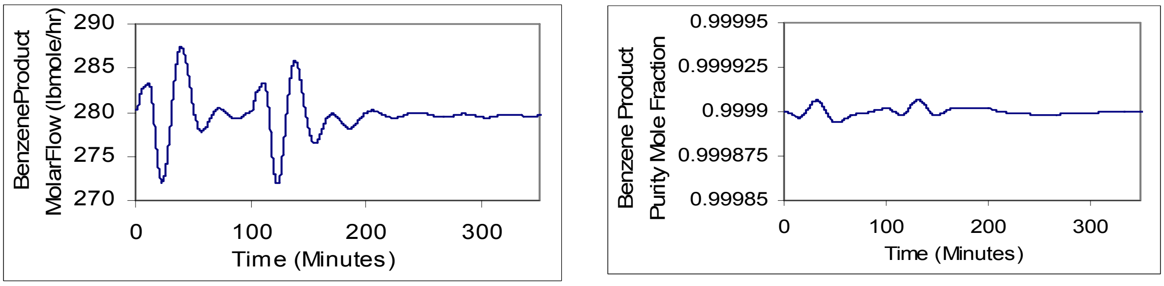


Figure 3.11: Rate of Accumulation of Toluene (thick line) and Benzene (thin line) During Load Disturbances in Toluene Feed Flow Rate

Feed Composition as Disturbance: Transient responses for production rate and product quality due to H_2 feed composition change from 0.95 to 0.925 at 100 min are given in Figure 3.12. Other process variables also settled within reasonable times. The variation in production rate and quality (Figure 3.12) is not significant because the ratio between H_2 and aromatics is controlled at the reactor inlet. So, though the feed quality changes, there is not much change in the production rate and quality.



(a) (b)

Figure 3.12: (a) Production Rate (b) Product Quality Variation due to Feed Composition Disturbance

Servo Tracking: The set-point of flash level control (FlashLC controller) is changed from 50% to 55% at 100 min, from 55% to 45% at 150 min and from 45% to 50% at 200 minutes. In all these cases, the controller is able to track the set-point quickly (Figure 3.13). The set-point change in the flash level control is an important plant-wide disturbance as it affects all the process variables in the separation section which in turn affect the process variables in the reaction section. In addition to the good servo tracking response all other process variables are also observed to be maintained at the desired set-points.

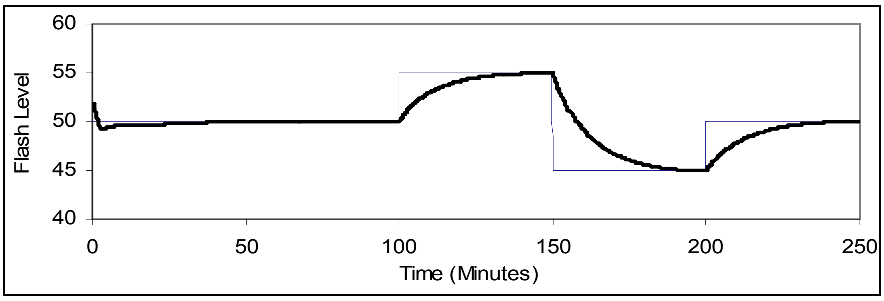


Figure 3.13: Set-Point Tracking Performance of Flash Level Controller: thick line - process variable and thin line - set-point

The use of rigorous nonlinear simulation is inevitable, whatever may be the methodology. Some previous studies employed it for validation purposes at the end and some other studies have not validated the resulting control system design via rigorous nonlinear simulation. This may lead to unworkable control systems. For example, Vasbinder et al. (2004) observed that the PWC systems developed by Stephanopoulos (1984) and Fisher et al. (1988) are infeasible. The proposed framework has the unique advantage of making the simulation an integral part of the control system design. This takes care of validation along with the development of a control system, which were done sequentially in all the previous methodologies.

3.6 Summary

An improved heuristic methodology is proposed by addressing the limitations associated with the 9-step heuristic procedure of Luyben et al. (1999). For example, more specific and yet generic guidelines are included which will facilitate the decision making for the throughput and inventory control. They will also aid the novices to understand the potential alternatives at each stage and choose the better one based on the process knowledge and requirements. The improved heuristic procedure is integrated with simulation as the heuristics cannot always be relied for PWC decisions. The proposed integrated framework is successfully applied to the HDA process. Results show that a viable control system can be generated by the proposed framework which synergizes the powers of both heuristics and simulation. The gist of the present work is that the control system design (especially for complex processes) cannot be accomplished just by heuristics without the aid of rigorous nonlinear simulation tools. It seems like common sense but it is worth repeating, especially in the context of PWC as researchers have so far not given enough attention to process simulators.

As a result of the application of the proposed integrated framework to the HDA process, it is seen that the conversion controller improves the overall performance. Though conversion controller appears to be somewhat less common, it is not uncommon in petrochemical processes. For instance, Turkay et al. (1993) proposed to use conversion controllers for all the three reactors in styrene manufacturing process to improve the PWC system performance.

CHAPTER 4

A SIMPLE AND EFFECTIVE PROCEDURE FOR CONTROL DEGREES OF FREEDOM*

The focus of this chapter is on one of the important steps in designing PWC systems, namely, CDOF. There appears to be no simple procedure to compute CDOF, the maximum number of flows that can be manipulated simultaneously, especially in the context of PWC of industrial processes. Hence, a simple and yet effective procedure to find CDOF is proposed and illustrated in this work. The key idea is to define 'restraining number' (i.e., the minimum number of flows that can't be manipulated along with others in an unit, which is also an inherent characteristic of that unit) of an unit. We show that the restraining number is equal to *the number of independent and overall material balances with no associated inventory*† in that particular unit. The concept of restraining number is then used to find CDOF of not only simple units but also highly integrated processes. One of the advantages is its generic nature, which facilitates its automation. Moreover, the proposed procedure implicitly takes care of number of phases and components involved in the unit. In addition, the proposed procedure needs just the basic understanding of simple units and one does not require all the mathematical equations involved.

* This chapter is based on the paper - Konda, N. V. S. N. M.; Rangaiah, G. P.; Krishnaswamy, P. R. A Simple and Effective Procedure for Control Degrees of Freedom. Chem. Eng. Sci. 2006, 61 (4), 1184-1194.

† Inventory is used here to refer to 'variable hold-up' but not 'fixed hold-up'. For example, gas phase (or gas-liquid phase) PFR is considered as the 'unit with inventory' as it contains 'variable hold-up' and liquid phase PFR is considered as the 'unit without inventory' as it contains 'fixed hold-up'.

4.1 Introduction

CDOF is the maximum number of streams that can be manipulated simultaneously, and is the first and foremost thing that needs to be computed during control system design as it determines the feasibility of the control system. Traditionally, control DOF is obtained by subtracting the sum of number of equations and externally defined variables from the number of variables (Seborg et al., 2004; Seider et al., 2004). This procedure is impractical especially for highly integrated plants and is prone to errors considering the large number of equations and variables present in the industrial processes. Luyben et al. (1999) proposed to count the number of control valves to find CDOF of the process. This is true but not a practical solution at the design stage because many a times the control engineer is required to place the control valves in the process flow diagram which, in turn, needs a priori knowledge of CDOF of the process. That means the CDOF needs to be known before placing the control valves. Then, the control valves can be placed in strategic locations in the plant. Else, it may so happen that more or less number of control valves may be placed if the engineer is not familiar with the plumbing rules. These kinds of problems occur more frequently if the process is highly integrated. Ponton (1994) proposed a method for CDOF by counting the number of streams and subtracting the number of extra phases (i.e., if there are more than one phase present in that unit). However, simple examples can easily be constructed where this method fails. For example, CDOF for a heater/cooler remains the same irrespective of the number of phases involved in that unit. Larrson (2000) also observed some cases wherein Ponton's (1994) method fails. In order to circumvent all of the aforementioned problems, an elegant way of computing the CDOF based on process flowsheet is developed and presented in this chapter.

The remaining chapter is organized as follows. Next section gives the theoretical background along with the application of the proposed procedure for many standard/simple units. Section 4.3 presents successful application of the proposed method to relatively complex units such as distillation columns. The proposed method is also successfully applied to several highly integrated processes of varying complexity in section 4.4. Finally, chapter summary is given in section 4.5. Application of the proposed method to additional industrial processes is given in the Appendix B.

4.2 Proposed Procedure

Design DOF has been extensively studied by several researchers in which the fundamental principle is the Gibb's phase rule (Gilliland and Reed, 1942; Kwauk, 1956; Smith, 1963). In contrast to the Gibb's phase rule which exclusively deals with the intensive properties, CDOF deals with extensive variables (i.e., flows). Hence, a procedure for CDOF just based on the extensive variables (i.e., based on the flows only without needing to write all the mathematical equations involved), as presented in this chapter, would be useful.

Whatever may be the nature of the control loop (flow, level, pressure, temperature or composition), ultimately the manipulated variable is going to be the flow rate of a process stream (including utility/energy streams as well). The question here is then can we manipulate all the process streams? If not, what is restricting us from manipulating some process streams? It is the nature of the equipment and/or process structure that restrains/limits the use of a particular flow as the manipulated variable. Mathematically,

Control DOF of an unit ≤ Total number of streams associated with that unit (4.1) *or*

Control DOF of an unit + X = Total number of streams associated with that unit (4.2)

where ‘X’ is the number of flows that cannot manipulated once the rest of the flows are selected as manipulators. We call ‘X’ the *restraining number* as it restrains the designer from using ‘X’ number of flows as manipulators. This is similar to *Restricting Relationships* introduced by Smith (1963) in the context of *Design DOF*. Now, equation 4.2 can be rewritten as follows.

Control DOF of an unit + *Restraining number* = Total number of streams associated with that unit (4.3)

Restraining Number: It is observed that CDOF may be different for any unit based on the flowsheet structure, but *restraining number* (the number of streams that can’t be manipulated) for any unit remains the same irrespective of the environment it is in. For example, for the simple mixer with ‘n-1’ input streams (Figure 4.1), CDOF varies with ‘n’ whereas the restraining number remains the same irrespective of the value of ‘n’. Hence, it can be concluded that the *restraining number* is the characteristic of the particular unit. We can find *restraining number* of each and every unit from the basic understanding of these units which is the objective of this section. This can then be used to calculate CDOF using equation 4.3.

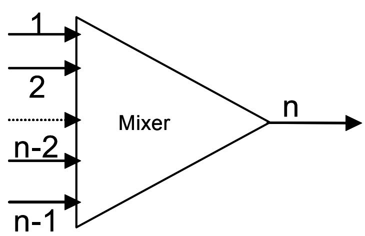


Figure 4.1: Mixer with (n-1) Inlet Streams and One Output Stream

Restraining Number of Standard Unit Operations without Inventory: The overall material balances restrict the total number of flows that can be manipulated simultaneously (i.e., once we manipulate certain number of flows, rest of the flows will be dictated by these balances). Component material balances can be ignored while computing CDOF of any unit, which simplifies the analysis to a great extent. This can be further justified by Pham's (1994) observation that the number of components has no role to play while computing CDOF once the inlet streams are fully specified. For example, consider an unit with no inventory (Figure 4.2). Units like mixer, splitter, valve, pump and compressor fall under this category. Overall material balance for such an unit can be written as

$$F_1 + F_2 + \ldots.. + F_{m-1} + F_m = F_{m+1} + F_{m+2} + \ldots.. + F_{n-1} + F_n \tag{4.4}$$

It can be seen that only 'n-1' flows can be fixed by the designer and the remaining flow will be given by equation 4.4. In terms of control, the minimum number of flows that the control engineer can't manipulate (restraining number) is 1 which is equal to the number of independent and overall material balances. In other words, the maximum number of flows that can be manipulated by the control engineer (CDOF) is 'n-1' which is equal to the difference between total number of streams and number of independent and overall material balances.

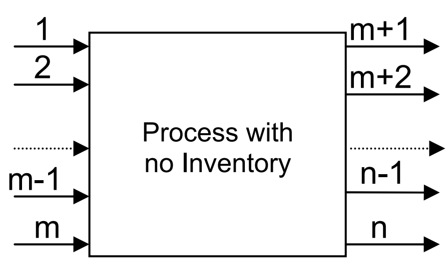


Figure 4.2: Generic Input/Output Structural Representation of Units without Inventory

More generally, it is possible to have more than one independent and overall material balance in an unit such as heat exchangers (generic representation shown in Figure 4.3).

$$F_1 + F_2 + \ldots\ldots + F_{m_i-1} + F_{m_i} = F_{m_i+1} + F_{m_i+2} + \ldots\ldots + F_{n_i-1} + F_{n_i} \quad (4.5)$$

where i = 1, 2, .., N, and N is the total number of overall and independent material balances. In this case, there exists N constraints (one for each overall material balance) and N flows can't be manipulated by control engineer. Therefore, only $\sum_{i=1}^{N}(n_i - 1)$ flows can be manipulated and so CDOF is $\sum_{i=1}^{N} n_i - N$, which is equal to the difference between total number of streams and total number of independent and overall material balances.

From the above analysis, restraining number for units with no inventory can be defined as:

Restraining number = Total number of Independent & Overall Material Balances (4.6)

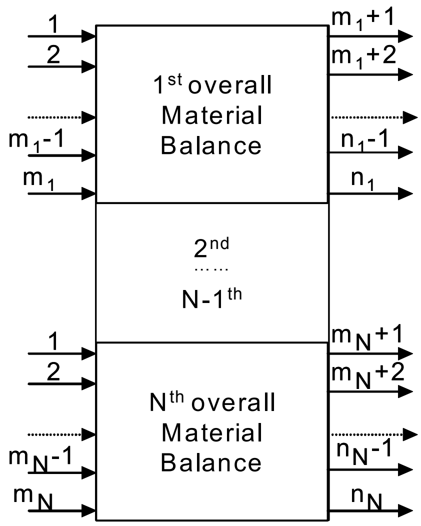


Figure 4.3: Generic Input/Output Structural Representation of Units with no Inventory but with Multiple 'Independent and Overall' Material Balances

Restraining Number of Standard Unit Operations with Inventory: The presence of inventory offers flexibility from control point of view. For example, in the case of mixer with no inventory (Figure 4.1), at least one flow can't be manipulated as it is dictated by overall material balance. However, in the case of a mixer with inventory (Figure 4.4), stream 3 can also be manipulated, say, to control level (inventory) in the mixer. So, in the case of units with inventory, restraining number is not only a function of total number of independent and overall material balances but also a function of number of inventories. The function depends on how the inventories are distributed among all the independent and overall material balances. However, specific relationship can be found based on the engineering judgment as discussed below.

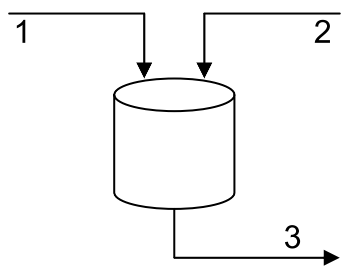


Figure 4.4: Mixer with inventory

In the case of units without inventory, it has been observed in the above analysis that the overall material balance does not allow control engineer to manipulate all the available process streams. However, in the case of units with inventory, process variables associated with inventories (for example pressure for vapor and level for liquid) offer additional flexibility from control point of view. If there exists an inventory associated with an overall material balance, in principle, it is possible to manipulate all the streams associated with that material balance either to control the extensive or intensive variables as long as we don't try to regulate all the extensive variables or all the intensive variables simultaneously. Controlling all the extensive variables violates overall mass balance (and leads to continuous accumulation which is not desirable) if there is any disturbance or error in measurements. Similarly, for any non-reactive system with fixed inlet composition, according to Duhem's theorem, specifying any two intensive variables completely specifies the system and so it is not possible to control all the intensive variables independently as they are dependant on one another.

For example, it can be seen from Figure 4.4 that the presence of inventory allows us to manipulate all the streams associated with it to control 2 extensive variables (say, flow rate of streams 1 and 2) and to control level (say, using stream 3 flow rate). Based on this, restraining number for units with inventories is given by

Restraining number = Total number of independent & overall material balances with no associated inventory (4.7)

Equation 4.7 reduces to equation 4.6 in case of no inventory, and is generic taking care of number of phases implicitly. Qualitative justification for this can be given: any additional phase, which in turn creates additional inventory, in the unit will automatically be associated with an outlet stream. Based on the discussion given above, this outlet stream can also be manipulated as it is associated with an inventory. As an example, consider a flash separator whose restraining number is zero as there are zero material balances with no inventory, irrespective of whether it is two- or three-phase separator (i.e., all the flows can be manipulated, which is true). All the standard units fall under two categories: units with overall material balances with associated inventory or without associated inventory. Then, CDOF of an unit can be calculated from equation 3 which is rewritten as:

Control DOF of an unit = Total number of streams associated with that unit – Restraining number of that unit (4.8)

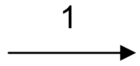
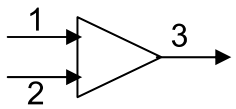
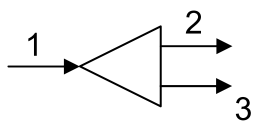
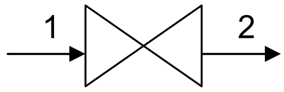
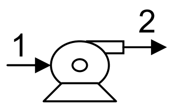
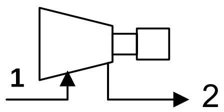
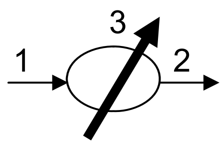
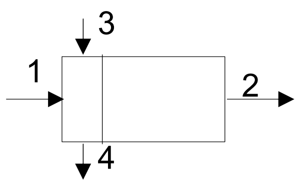
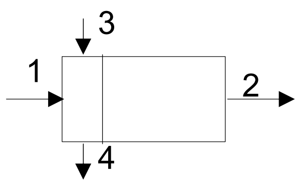
Table 4.1 gives the restraining number (from equation 4.7) and CDOF (from equation 4.8) for several standard units. For other operations and/or situations, which are not covered in Table 4.1, equation 4.8 can be used to obtain the corresponding CDOF. In this table and subsequent figures, thick and thin lines represent energy and material streams respectively.

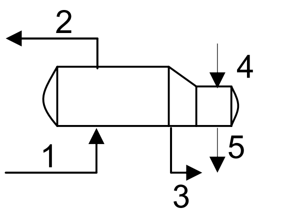
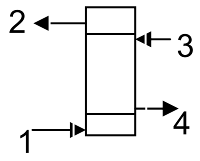
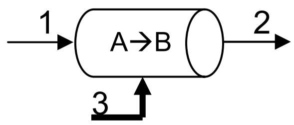
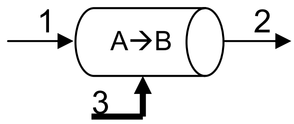
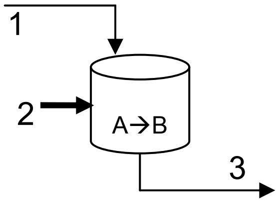
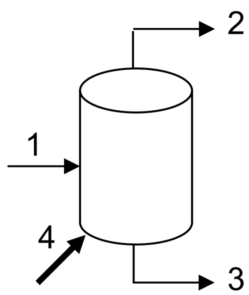
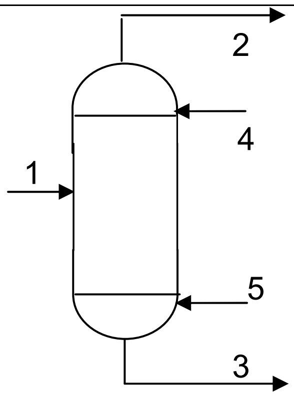
The power of the proposed method can be seen when it is applied to relatively complex and highly integrated processes. For such a process, CDOF is given by

Control DOF for a process = Total number of streams in that process – Sum of the restraining numbers for all the units in that process (4.9)

This is proved by considering a few simple and yet typical processes.

Table 4.1: Restraining Number and CDOF for Several Standard Units

Stream/Unit	Schematic Representation	Overall Material Balances with No Associated Inventory	Restraining Number (Eq. 7)	Total Number of Streams	CDOF (Eq. 8)
Material/Energy Stream		-	0	1	1
Mixer		$F_1+F_2=F_3$	1	3	2
Splitter		$F_1=F_2+F_3$	1	3	2
Valve		$F_1=F_2$	1	2	1
Pump		$F_1=F_2$	1	2	1
Compressor		$F_1=F_2$	1	2	1
Heater/Cooler, Furnace		$F_1=F_2$	1	3	2
Heat Exchanger, Condenser (Total/Partial)		$F_1=F_2$ $F_3=F_4$	2	4	2
Flooded Condenser		$F_1=F_2$	1	4	3

Kettle Reboiler		$F_4=F_5$	1	5	4
Vertical Thermosyphon Reboiler with steam on shell-side		0	0	4	4
Gas Phase PFR (Non-adiabatic)*		0	0	3	3
Liquid Phase PFR (Non-adiabatic)*		$F_1=F_2$	1	3	2
CSTR (Non-adiabatic)*		0	0	3	3
Flash (Non-adiabatic)*		0	0	4	4
Tray/Packed Column (excluding reboiler and condenser)		0	0	5	5

* For adiabatic units, energy stream will be absent and correspondingly both the total number of streams and CDOF will less by one.

According to equation 4.9, CDOF for the process in Figure 4.5(a) is calculated as 4, which is true because it can be easily seen from this figure that all the 4 flows can be manipulated simultaneously either to manipulate extensive or intensive process variables. For the process in Figure 4.5(b), CDOF using equation 4.9 is 4, which is true as can be seen from that figure. So, it can be concluded that the restraining number concept to compute CDOF is equally valid even for complex processes. It can be further justified based on the generic nature of the restraining number as it remains the same irrespective of the environment the unit is in, say, as a simple unit or as an integral part of a highly integrated process. Moreover, the proposed procedure for CDOF involves the total number of streams in the process which automatically accounts for the change in the number of streams with process structure. For example, consider direct feeding of streams 1 and 4 to the reactor without the mixer in Figure 4.5(b); it is obvious that CDOF is still 4 as all streams (1, 3, 4 and 6) can be manipulated. The change in process structure is automatically taken care by equation 4.9. As the total number of streams is less by one (due to the absence of stream 2) and the total restraining number is also less by one (as the restraining number associated with mixer will not be there anymore), CDOF remains the same.

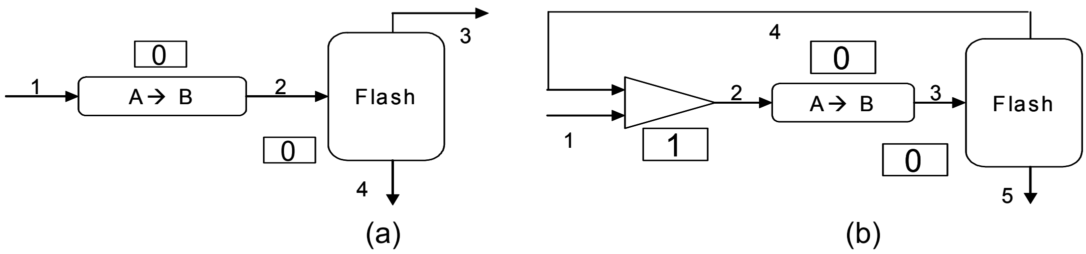


Figure 4.5: Gas-Phase Reactor and Flash (both Adiabatic): (a) without Recycle and (b) with Recycle. Restraining Number of the Unit as per Table 4.1 is shown in the rectangular box near it.

Procedure: To find CDOF of complex processes, number each and every stream (including energy and utility streams) in the process flow diagram. Place the *restraining number* of each unit (based on Table 4.1) inside/near that unit as shown in Figure 4.5. CDOF of the process can now be calculated by subtracting the sum of the restraining numbers of all the units from the total number of streams (including energy and utility streams) in the entire process (equation 4.9). This procedure can appropriately be called as *Flowsheet Representation of CDOF* as it uses just the flowsheet information. As noted before, restraining number concept to calculate CDOF is applicable to any process irrespective of the number of phases and components in the process as long as the process is feasible. It is equally valid even for solids handling systems (such as cyclones, grinders, filters).

The CDOF can be obtained by adapting the concept similar to the one proposed by Rudd and Watson (1968) in the context of Design DOF, which can be written as:

$$\text{CDOF} = \sum_{\substack{\text{Over all}\\ \text{the units}}} \begin{pmatrix} \text{number of} \\ \text{independent} \\ \text{handles over} \\ \text{an unit} \end{pmatrix} - \text{number of streams which are interconnected between two units.} \quad (4.10)$$

The proposed procedure for CDOF has an unique advantage over this procedure. The number of independent handles over an unit may change with the process structure in the above formula. But the restraining number for an unit remains the same irrespective of the number of phases, inputs and outputs involved. For example, the number of independent handles for a mixer (splitter) may change with the number of inlet (outlet) streams. However, the restraining number for a mixer (splitter) remains the same irrespective of the number of inlet (outlet) streams. So, the proposed procedure is more generic and can be automated easily.

The above analysis on CDOF did not include any mechanical means of manipulation such as the mechanical agitator in reactors which is usually driven by a variable speed motor to vary the reaction rate to control the required process variable. For example, the TE process (Downs and Vogel, 1993) has one mechanical

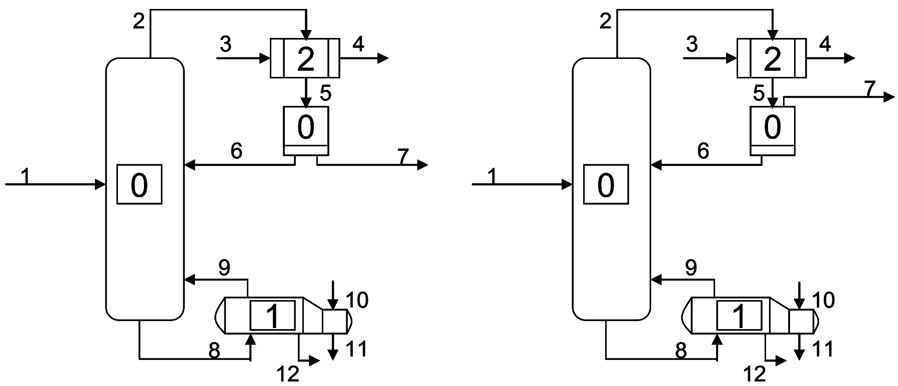
CDOF. So, CDOF should be increased by the corresponding number of mechanical manipulators whenever available. In addition, it should be noted that the proposed analysis for CDOF deals only with the process flows which can be manipulated (using a control valve) simultaneously. The analysis has not considered any pressure reduction valves which are used to set the pressure at a down-stream location. However, pressure reduction valves can be placed on any pipeline as per process requirements, even if the flow is being manipulated (because of the inherent relationship between valve opening and pressure drop). Hence, the CDOF obtained by the proposed procedure will increase by one for each pressure reduction valve present in the process. Based on this, equation 4.9 can be updated as follows:

Control DOF for a process = Total number of streams in that process – Sum of the restraining numbers for all the units in that process + The number of mechanical or any other manipulators other than the process flows (such as agitators) and the number of pressure reduction valves (i.e., the valves used exclusively for pressure reduction) 4.11

It is important to note that CDOF gives *the maximum number of flows that can be manipulated simultaneously* whereas the minimum number is dictated by stability considerations. Actual number of manipulated variables (i.e., control valves) is between the minimum number and CDOF. For example, minimum number of manipulated variables for a distillation column (with condenser and reboiler) is 3 in order to maintain its stable operation i.e., to control pressure, accumulator level and level in the sump (in case of thermosyphon reboiler) or in kettle reboiler. On the other hand, as discussed in the following section, CDOF for this column is 6. The additional 3 manipulated variables can be used for feed flow (which can be considered either as a disturbance or as a manipulator), top and bottoms compositions. Based on the process requirements, control engineer would go for single or double end composition control. The CDOF of distillation column is further discussed in the following section.

4.3 Application to Distillation Columns

Application of the proposed procedure to distillation columns needs special care because of close and complex interconnection of several units in a column, which is typically a combination of tray/packed section, condenser (total condenser in Figure 4.6(a); partial condenser in Figure 4.6(b)), reflux drum and a reboiler. As stated above, the proposed procedure holds good even for a combination of several units. Hence, it is applied to this distillation column. Restraining numbers of tray/packed section, condenser, reflux drum and reboiler are shown in Figure 4.6. Since there are a total of 12 streams, CDOF according to equation 4.9 is 12 – (2+1+0+0) = 9. However, CDOF is usually said to be 6 for a standard distillation column shown in Figure 4.6. Does this mean the proposed procedure fails in case of distillation columns? No. As mentioned earlier, the complex behavior of distillation column along with its requirements puts additional restrictions. This can be explained based on redundancy in process variables that need to be controlled.



(a) (b)

Figure 4.6: Distillation Column with (a) Total Condenser and (b) Partial Condenser

Redundancy in pressure-related process variables in the distillation column overhead section: In the case of total condenser (Figure 4.6(a)), it is possible to manipulate streams 2 and 3 simultaneously when tray/packed section and condenser are considered as separate units. When these units are put together, they can still be manipulated simultaneously to control pressure at the top of the column and in the condenser. However, pressure drop between column top and condenser is usually negligible and so the pressure in the top of the column and in the condenser can be considered as a single process variable. This means, manipulating either stream 2 or 3 should be sufficient to maintain the pressure at the desired value. On the other hand, manipulating both streams 2 and 3 to control pressure in the column top and condenser is going to be very difficult, if not impossible, as these controlled variables are very close and interact with each other. Moreover, the additional pressure drop that would be introduced by placing the valve on stream 2 makes it economically less attractive. So, it is not a good idea to use two manipulators while one manipulator can serve the purpose. The choice between stream 2 and 3 here depends on the nature of the dynamics. If the pressure dynamics is fast or the column is fairly small, stream 2 is usually considered as the manipulator else stream 3 will be the manipulator.

In case of a partial condenser (Figure 4.6(b)), in addition to streams 2 and 3, there is one more alternative to control pressure by using stream 7. As mentioned earlier, one amongst these three streams (2, 3 and 7) should be sufficient to maintain the pressure in the column; and the choice depends on the nature of the pressure dynamics. In case of horizontal flooded condenser, with process fluid on the shell side, stream 5 is another potential manipulator to control the operating pressure in the distillation column (by maintaining the level in the condenser which in turn varies the surface area available for heat transfer). Thus, number of alternatives to control the operating pressure has increased but not the process variables as such. In the case of vertical flooded condenser where the process fluid is usually inside the tubes, we can't manipulate stream 5, but coolant flow (stream 3) can be manipulated to maintain the coolant level on shell side to vary the heat transfer area which in turn maintains the pressure.

Redundancy in level-related process variables in the distillation column with kettle reboiler: The sump level and the reboiler level can be controlled if they are considered as independent units. They can in principle be controlled simultaneously even when they are put together. However, when they are considered together, the sump level is redundant and need not be controlled explicitly because the mechanical design ensures that the sump level is maintained all the time by virtue of constant level (because of the baffle) in the reboiler. There are two fundamental reasons which make the sump level self-regulating. If there is any disturbance and the sump level is increasing, then (1) because of the increased static pressure the flow will be more at the bottom of the column to the reboiler as it is based on natural circulation where the flow is a function of static head and (2) because of the increased static pressure the bubble point of the bottoms stream will rise and vaporization will be less thus reducing the reboiler pressure which creates hydrostatically unbalanced system momentarily. The cumulative effect of these two factors forces the flow over the baffle more (in to surge) and boil-up rate less. Owing to the latter, density of fluid on trays in the column will rise and overflow over the weirs will be less which in turn decreases the sump level till it reaches the original value, to return to the hydrostatic balance between the sump level and static head held by baffle. There is a possibility of inverse response in the bottom sump level. However, for the sake of simplicity in the analysis, this is not mentioned in the above reasoning. The principle here is similar to the hydrostatic balance in an U tube except that the analysis is more complex because of the interaction between material and energy. Similar reasoning can be given even if there is a disturbance which reduces the sump level.

Based on the above discussion, the sump level is a redundant process variable from control point of view as it is hydrostatically balanced because of the static head held by baffle in the reboiler. Of course, the distillation bottom section and reboiler should be properly designed else flooding can easily take place. For example, mechanical design decisions such as the spacing between the sump level and vapor entrance nozzle at the bottom of the column and the space above the baffle in the kettle reboiler for liquid disengagement should be properly chosen to easily resume hydrostatic balance in the system and to avoid flooding.

Redundancy in pressure-related process variables in the distillation column with kettle reboiler: Pressure in a kettle reboiler can be a process variable when it is alone (though it is not usual practice to control the pressure in the reboiler, it is theoretically possible). Once it is part of a distillation column, pressure control at the top of the column would ensure the pressure in the other parts and there is no need to control the pressure in the reboiler. Hence, this is also a redundant pressure-related process variable.

In view of above 3 redundant process variables, the effective CDOF is only 6 (= 9 - 3) which is usually the case. So, in the following cases, the restraining number for a distillation column (with total/partial condenser and with kettle reboiler) is increased by 3 to account for the 3 redundant process variables. In the case of distillation columns with internal reboilers/open steam, the redundancy is only one which is associated with the pressure-related process variables in the overhead as there are no redundant process variables at the bottom of the column. Distillation columns with thermosyphon reboiler of any configuration (vertical or horizontal; with or without baffle in the sump; Sloley, 1997) can be analyzed similar to that of the distillation column with kettle reboiler to find the redundancy before applying the concept of restraining number to compute the effective CDOF. For example, in the most commonly used thermosyphon reboiler (i.e., vertical with steam on shell side), the process stream that comes out of reboiler can, in principle, be manipulated to control the pressure. However, as discussed in the case of kettle reboiler, it is not required to control the pressure in the reboiler and hence this manipulated variable is redundant. For complex distillation columns with additional side draws, which are very common in petroleum refineries, each side draw increases the CDOF (by using equation 4.9 and redundancy) by one and the proposed procedure will automatically manifest this without any additional considerations.

4.4 Application to Complex Integrated Processes

In this section, the *restraining number* concept is applied to several highly integrated processes of varying complexity to prove its applicability. The resulting CDOFs are validated by comparing them with those available in the literature. For the process in Figure 4.7, CDOF (from equation 9 and the concept of redundancy) is 6 [= Total number of streams – (Sum of restraining numbers of all units + Number of redundant process variables associated with stripper) = 9 – (1+2)]. According to Luyben (1996), CDOF is 4. However, he presumes constant temperature in the reactor and constant pressure in the stripper which contribute two more variables to CDOF. So, total CDOF is 6 which is the same as that obtained by the proposed procedure. In subsequent applications (including those in the Appendix B) total CDOF from Luyben (1996) is considered for comparison. From Table 4.2, it can be seen that the proposed procedure is successful in predicting the CDOF of highly integrated processes in Figures 4.8 and 4.9 correctly. All the reactors in Figure 4.8

are assumed to be of CSTR type whereas Westerberg process (Figure 4.9) contains a gas-phase PFR.

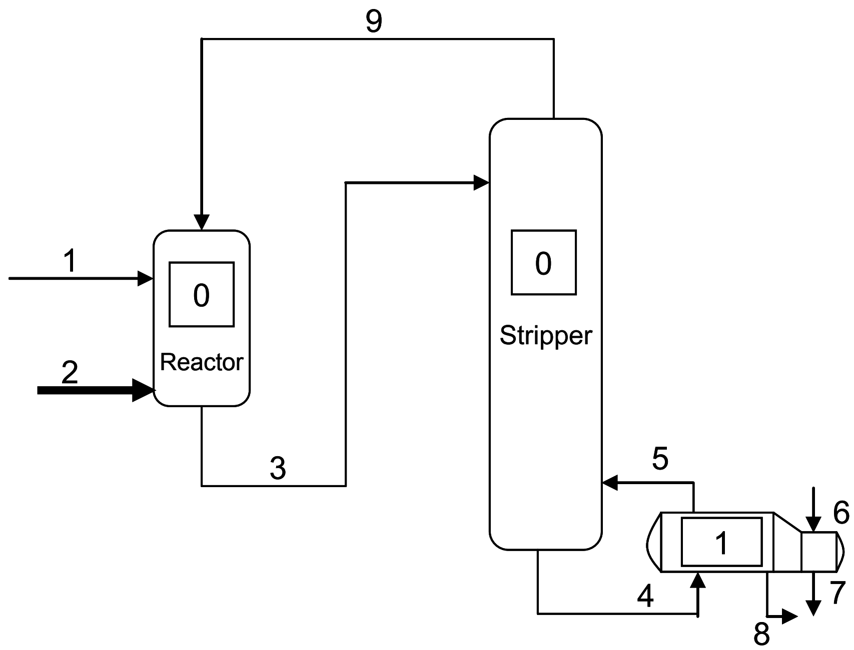


Figure 4.7: Reactor (CSTR)/Stripper Binary Process with One Recycle

Table 4.2: CDOF for Processes shown in Figures 4.8 and 4.9

Figure Number	CDOF from Equation 9 and the Concept of Redundancy	Total CDOF from Luyben (1996)
4.8	24 [= 42 - (2+1+2+1+2+1+3×3)]	24
4.9	6 [= 9 – (1+1+1)]	6

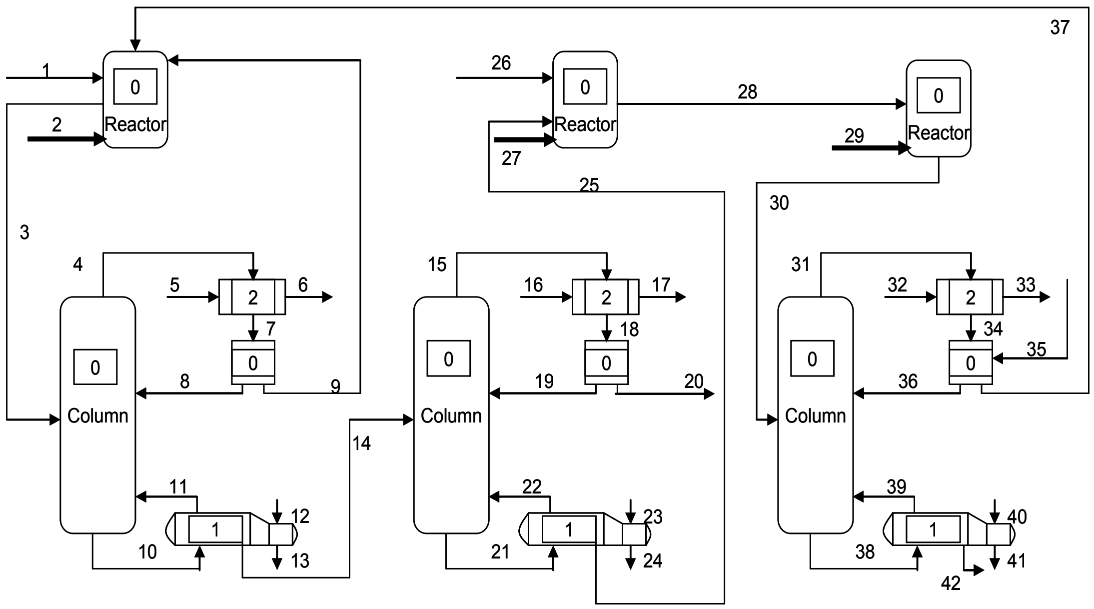


Figure 4.8: Luyben Challenge Process (Luyben, 1996)

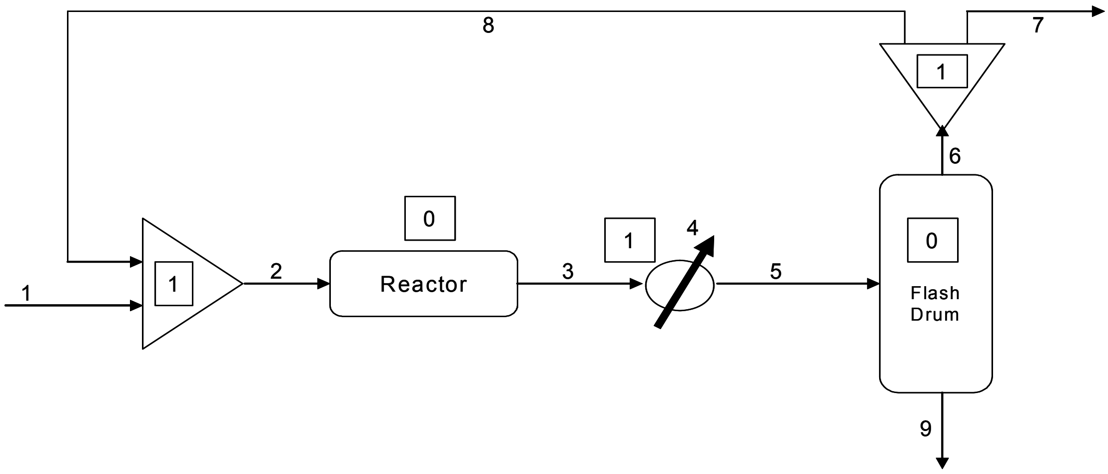


Figure 4.9: Westerberg Process (Luyben, 1996)

Flowsheet Representation of CDOF, as developed above, has several other advantages:

1. Many times, control engineers prefer working with subsystems of the plant (especially in the initial stages of developing control system for new and/or complex processes). Then it is necessary to re-compute the CDOF for that particular section. By making use of the proposed '*Flowsheet Representation of*

CDOF', re-computation of the CDOF for that section can be avoided. It can directly be accessed from the flowsheet once it is done.

2. The only information that is needed to build this *Flowsheet Representation of CDOF* is some basic knowledge of CDOF of simple units. The only prerequisite is that the process design must be feasible.
3. The flowsheet representation implicitly takes care of the number of components and phases involved in the process thereby reducing the complexity involved in the computation of CDOF.
4. Overall CDOF gives the maximum number of control valves that can be placed in the entire plant. But it does not tell anything about the maximum number of control valves that can be placed around an unit. It may then be possible that, though the overall CDOF is satisfied, the CDOF of an individual unit is not met. By adapting the proposed procedure, both the overall CDOF and the CDOF of individual unit can be fulfilled.

4.5 Summary

Restraining number, a characteristic feature of an unit, is proposed; it is equal to the total number of independent and overall material balance equations with no associated inventory. Restraining number for several simple units is computed from the basic understanding of their functioning. In case of complex units like distillation columns, the concept of redundancy is demonstrated. These are then used to compute CDOF of highly integrated processes. The proposed procedure for CDOF gives the maximum number of flows that can be manipulated simultaneously in a process, and the control engineer can avail some (or all) of them based on process characteristics and requirements. It can be automated and implemented in process simulators very easily because of the generic nature of the restraining number. The proposed procedure is clearly simpler than the conventional "variables minus equations" approach as it just needs fundamental understanding of simple units even for highly integrated processes.

CHAPTER 5

PERFORMANCE ASSESSMENT OF PLANT-WIDE CONTROL SYSTEMS*

Performance assessment of control systems has been receiving growing attention in the recent past to improve operability and profit margins of the process. However, such studies, and also the tools available to carry out such studies, from plant-wide perspective are rather limited. In this regard, a new dynamic performance index called DDS is proposed in this chapter. It is then used to assess the performance of three PWC structures (CS1, CS2 and CS3) for the HDA process. The three control structures are distinctly different from the TPM standpoint: CS1 uses internal manipulator (e.g., reactor temperature), CS2 uses fixed-feed control strategy with balanced nature, and CS3 uses on-demand control strategy to control the throughput; consequently, rest of the control structure decisions are significantly different. By critically analyzing the results from rigorous nonlinear dynamic simulations, CS3 is observed to be exhibiting poorest overall dynamic performance. The plant-wide dynamic performance of CS2 is found to be superior or comparable to that of CS1 for all the anticipated disturbances. The analysis of the results reveals the effectiveness of DDS and rigorous simulation tools for PWC studies.

5.1 Introduction

Performance assessment of control systems has been an active research area for the last 15 – 20 years. Such studies from plant-wide perspective, however, are relatively limited mainly due to the complexity involved in PWC due to the

* This chapter is based on the paper - Konda, N. V. S. N. M.; Rangaiah, G. P. Performance Assessment of Plant-Wide Control Systems of Industrial Processes. Ind. Eng. Chem. Res., 46, pp. 1220-1231. 2007.

presence of dozens of process variables; to complicate the matter further, recycles, that are becoming common in chemical processes, are notorious for furthering process complexity by increasing not only the interactions among process variables but also process nonlinearity. Besides, the use of rigorous process simulators for PWC studies is even more limited as it is more tedious and computationally intensive to carry out such rigorous studies. In addition, performance assessment metrics which can easily and effectively be used in PWC studies based on rigorous process simulators are not available. Thus, in the present study, we propose a performance metric and then use it to evaluate three PWC systems for the HDA process.

Due to the large number of process variables in any PWC problem, there exists numerous alternative control structures. Controllability measures such as RGA, NI, CN, DCN, RDG, PRG, and CLDG have been very useful to screen off some control structures especially during the initial stages of control system design. However, after the initial screening, a handful of alternatives will be left which needs more rigorous analysis for the final selection. This can be done by simplified/linear dynamic simulation as commonly done by most of the researchers in the past; though, some researchers (e.g., Luyben, 2002) have been using rigorous nonlinear dynamic simulators for some years.. However, due to the increasing use of recycles in the chemical process industry, the processes are becoming more complex and their dynamics can be highly nonlinear (Kumar and Daoutidis, 2002). Consequently, there is a need to use rigorous nonlinear dynamic simulation, especially in the final stages of control system design, to make the analysis more realistic (Kim et al., 2000). In addition, some of the aforementioned metrics may not always yield reliable results; He and Cai (2004) presented several case studies in which control configuration design based on RGA and NI has failed. Similarly, Georgakis et al. (2003) presented an operability measure which is more consistent than the metrics such as RGA and CN.

At times, some of the above mentioned controllability measures cannot be used due to the complexity of the process at hand. Noting this, Yi and Luyben (1995) proposed a metric called steady-state disturbance sensitivity (SDS) based on steady-state to screen the control structures; the basic idea here is to compute the changes in the MV in the presence of disturbance(s) for different control structures. The control structure that requires larger changes in MVs is not recommended as it is more prone to hit constraints and valve-saturation limits. However, this measure cannot be always used: consider two control structures, C1 and C2. If the required changes in all the MVs in C1 are larger than that of C2, by making use of this measure, the decision is obvious, i.e., C2 is better. However, if some MV changes in C1 are less than that of C2 and the rest of the MV changes in C1 are more than that of C2, the decision is less obvious. Besides, SDS does not consider the performance during transient state and does not guarantee stability.

The use of any of the above tools is necessary but not sufficient, and should subsequently be complemented with rigorous dynamic simulation. But, as mentioned previously, in case of complex processes, such an analysis using nonlinear dynamic simulations can be very difficult and computationally intensive due to the presence of hundreds of control loops in a typical PWC system. Though, in principle, it is possible to compare the performance of each individual loop, it is very tedious. At times, there may not be any meaningful loop-to-loop comparison as a controlled variable in one control structure need not necessarily be controlled in another control structure. Alternatively, one might want to assign weights to each control loop to quantify the overall performance into a single index. But, the weights are often subjective.

The rest of the chapter is organized as follows. The next section discusses some of the common measures (in addition to the ones discussed above) and the associated problems, and then presents the proposed metric to assess the performance of PWC systems using rigorous simulation tools. Section 5.3 gives brief overview of the HDA process and its steady-state simulation. Implementation of three control structures for the HDA process in HYSYS is described in section 5.4. Their performance is then critically analyzed (using rigorous nonlinear dynamic simulation) in the presence of several anticipated disturbances in section 5.5. Finally, chapter summary is given in section 5.6.

5.2 Plant-Wide Performance Assessment Measures

Elliott and Luyben (1995, 1996 & 1997) proposed capacity-based approach to measure the dynamic performance of alternative control structures by computing the loss in capacity due to off-spec production; the measure is thus related to product quality regulation. Though capacity-based approach is a useful and practical measure, it cannot be applied in all situations. For example, in this approach, the off-spec product is assumed to be disposed. However, it may be economical to recycle it as the raw materials are usually expensive. Otherwise, yield-losses and additional costs due to disposal of the off-spec product may render the process uneconomical. Though it is possible to implement this feature in the capacity-based approach, it cannot be generalized. For example, it may not be desirable to recycle the over-purified off-spec product (although the under-purified off-spec product needs to be recycled) as it unnecessarily incurs additional costs. Even if the off-spec product has to be recycled, the recycling location and reprocessing costs will be process-specific. If the off-spec product is due to light impurities, it has to be recycled back to the light-component (impurity) purification section else it has to be processed through the heavy-component (impurity) purification section. At times, the off-spec product cannot be recycled due to capacity limitations (Zheng and Mahajanam, 1999;

Mahajanam and Zheng, 2002) but has to be stored (for future processing) which incurs additional inventory costs. Thus, reprocessing cost of the off-spec product will be different in each of these cases, and no generally accepted procedures are available to estimate it. One can assume some cost, but the results will be dependent on this assumed value.

Product quality is important, but it cannot be the sole measure. For example, using capacity-based approach and product quality as the measure, two alternative designs will be dynamically equally good if both are capable of producing on-spec product. However, this need not necessarily be true always. Consider product quality regulation in case of alternatives CS2 and CS3 (yet to be discussed in sections 5.4 and 5.5); there is essentially no difference in this regulation of product quality in the presence of uncertainty in the reaction kinetics (Figure 5.1, left). However, the same disturbance has significantly different impact on dynamics of the two alternatives (Figure 5.1, right). Hence, product quality regulation is only a necessary condition but not sufficient to be considered as an overall process performance measure. Similar example is presented in Chapter 6 (Section 6.3.1) to show the inadequacy of product quality as the overall performance measure. In addition, the ultimate decision on relative performance is likely to be biased on the performance of the product quality loop (i.e., its manipulator and tuning) if one uses capacity-based approach as the overall performance measure. In a similar way, the production rate also cannot be an appropriate measure for the overall performance. For example, on-demand control has better product-regulation capability, but its dynamics in the other parts of the plant are much slower and thus dynamic performance is not as good as a fixed-feed control strategy (Luyben, 1999).

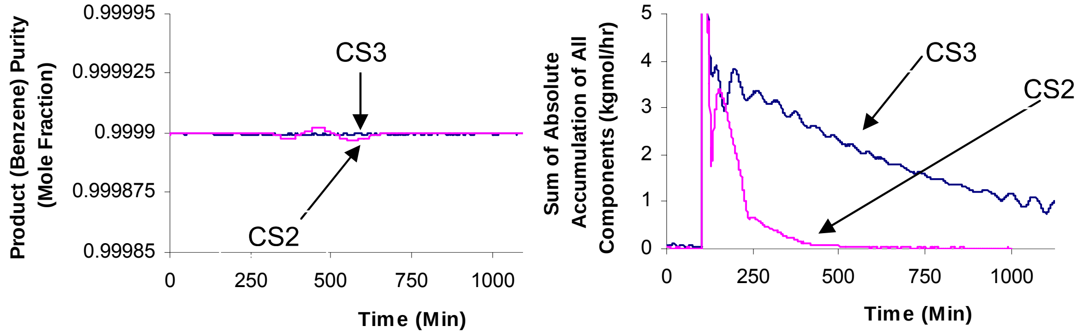


Figure 5.1: Product Quality (left) and Accumulation (right) Profiles for the HDA Process with CS2 and CS3 in the presence of Uncertainty in Reaction Kinetics

Sometimes, process settling time (i.e., time to reach steady-state after the process is affected by a disturbance) is used as a dynamic performance measure, especially in the presence of deterministic disturbances; the lower the settling the better is the control system. However, this measure ignores what is happening during the transient state (e.g., how far the process variable is from the steady-state value) and hence cannot be a good measure for dynamic performance. Figure 5.2 shows the accumulation profiles for -5% change in the throughput for the process with CS1 but with different TPMs – reactor temperature ($T_{R\text{-in}}$) and total toluene flow in the liquid recycle loop (F_R); based on the settling time, both the TPMs are equally good as their settling times are comparable (~ 200 min). However, during the transient, the impact on the process is much larger if $T_{R\text{-in}}$ is used as the TPM and thus the process becomes more sensitive, which makes $T_{R\text{-in}}$ a less attractive TPM; detailed discussion on the TPMs for CS1 is given in section 5.5. Thus, a good and comprehensive measure should include the information on process variables during transient along with settling time and also be able to capture this information over the entire process (i.e., from all the sections in the plant); this is precisely the subject of this chapter.

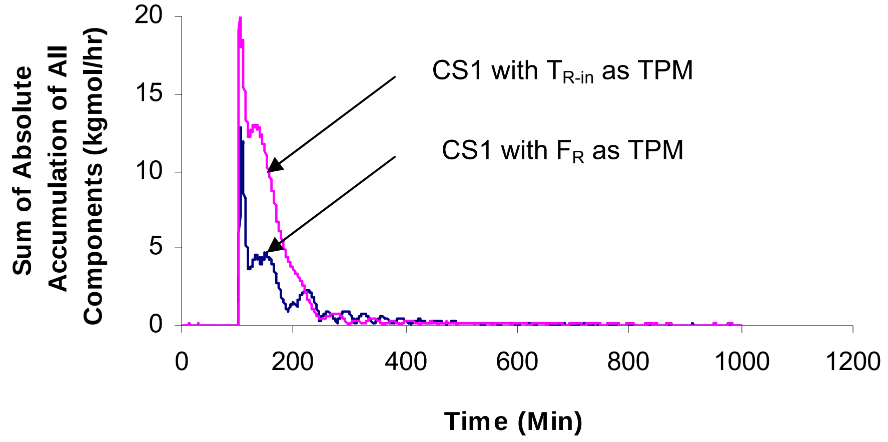


Figure 5.2: Accumulation Profiles for -5% Change in Throughput

5.2.1 Dynamic Disturbance Sensitivity (DDS)

In order to circumvent the difficulties discussed above, a new performance index is proposed in the present study. Through extensive simulations, we have identified that the overall control system performance and component accumulation (or depletion; i.e., rate of change) are strongly correlated. In the presence of disturbances, accumulation is not equal to zero for a certain period of time until the effect of disturbance is attenuated by the control system. Obviously, the process does not reach steady-state until and unless the accumulation is zero. Indeed, all controlled variables (and thus the associated manipulated variables) in the process are observed to reach steady-state if and only if the rate of accumulation of all components reaches zero. In addition, from Figures 5.1 and 5.2, it is evident that the effect of the disturbance on the process can be captured by accumulation profiles whereas product quality and settling time failed to serve as overall performance metrics. Thus, the integral of absolute accumulation can serve as a better measure to gauge the impact of disturbance on the process. Absolute accumulation is considered since neither a positive nor negative (i.e., depletion) value is desirable. Consequently, sum of absolute accumulation for all components is plotted and the area under the curve is used as a measure of PWC performance. Naturally, the lesser the area, the better is the control and the corresponding alternative. As this measure essentially quantifies the effect of disturbance on the process dynamics, it will be referred as “Dynamic Disturbance Sensitivity (DDS)” and is defined as

$$DDS = \int_{t=0}^{t_S} \left(\sum_{i=1\,to\,n} \left(absolute\ accumulation\ of\ component\ i \right) \right) dt \tag{5.1}$$

where t_s represents time taken to reach steady-state and n represents total number of components involved in the process. Accumulation is computed using the standard definition:

accumulation = input – output + generation – consumption (5.2)

where all the terms are based on ‘rate of change’. From the definition of DDS (i.e., sum of absolute errors in component material balances), it is similar to the other metrics (such as Integral Absolute Error, i.e., IAE).

The proposed DDS has several advantages as discussed below:

1. It is easier to compute DDS for a process with relatively less number of components than the number of loops, which often occurs; and data management and storage will also be less demanding for calculating DDS for such a process.
2. Procedure to compute DDS remains the same for a given process flow sheet even if the control structure changes. This feature can be very handy for analyzing performance of a large number of control structures and facilitates easy automation of the procedure. The procedure can be further simplified by ignoring some components present in insignificant quantities, as will be shown in the Section 5.

3. Unlike any of the steady-state based counterparts, there exists strong correlation between the value of DDS and process stability, as DDS is computed based on dynamics; for an unstable system, DDS will be very large.
4. DDS is more realistic as it considers level and pressure effects on dynamics which have not been considered in the other measures based on steady-state information.
5. In addition to screening alternative control structures, DDS can be used to compare alternative process designs; this aspect is discussed in Chapter 6. Furthermore, the relative impact of a disturbance on different sections of the plant can be quantified using DDS.
6. It can be easily combined with rigorous nonlinear simulation models. This not only improves the accuracy but also saves time as one does not have to linearize the process models in order to make use of linear model-based controllability indexes to analyze the performance.
7. DDS is equally applicable to performance analysis for set-point changes.
8. DDS is very useful to assess the dynamics of the process (such as overall time constant) without having to examine all the process variables to identify the slowest-responding one, which is dependent on several other factors (e.g., type of disturbance).
9. Due to the fundamental nature of the DDS, it can be used even as an open-loop controllability metric.

5.3 Process Description and Simulation of the HDA Process

For detailed information on the HDA process, refer to section 3.3.1 in Chapter 3. For a quicker and easier reference, process flow-sheet is given here (Figure 5.3) along with the reactions involved and fluid package used. Two main reactions taking place inside this reactor are:

Toluene + H_2 → Benzene + Methane

2 Benzene ↔ Diphenyl + H_2

The Peng-Robinson (PR) equation of state is selected for property estimation as it is very reliable for predicting the properties of hydrocarbons over a wide range of conditions and is generally recommended for oil, gas and petrochemical applications.

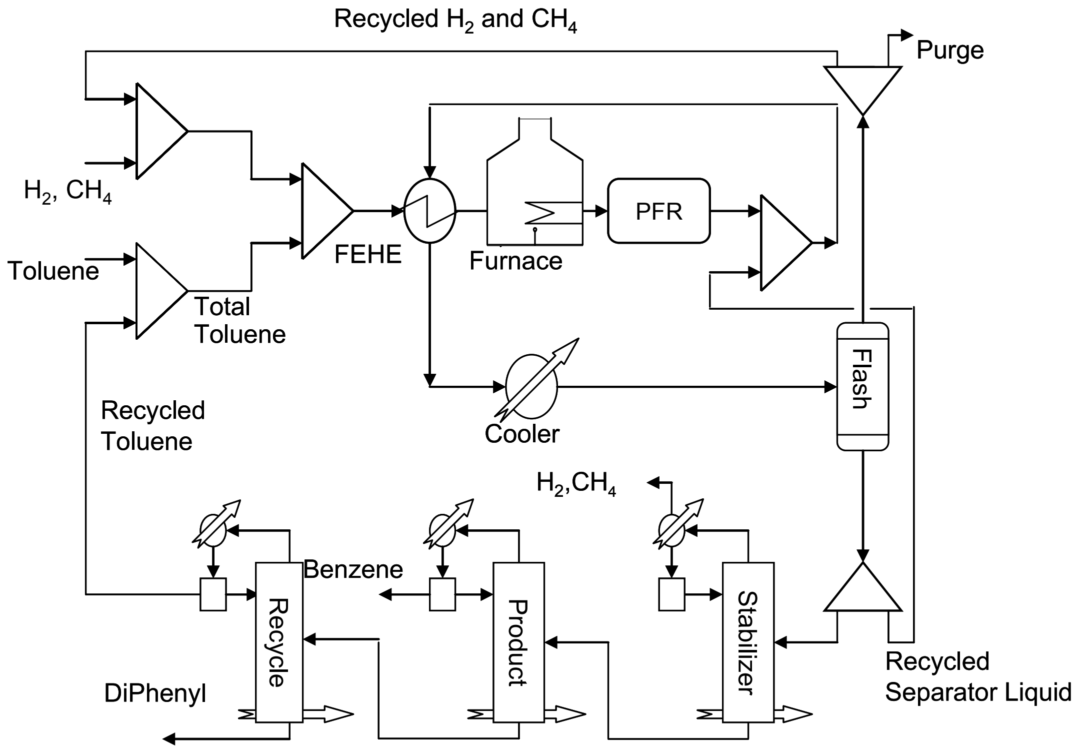


Figure 5.3: Flow-Sheet of the HDA Process to Produce Benzene from Toluene

5.4 Dynamic Simulation of PWC Systems for the HDA Process

There has been increasing number of studies on PWC and several methodologies have been proposed. However, there has not been any comparison of these methods so-far. Thus, instead of randomly choosing the control structures, we have chosen the candidate control structures resulting from different PWC methods. Hence, the present study brings out the relative merits of different PWC methodologies also. Several researchers have proposed different control structures for the HDA process using their own methodologies. One of the popular PWC methodologies is the heuristic procedure by Luyben and co-workers, and this method was applied to the HDA process to develop PWC structure (Luyben et al., 1999). The resulting control structure is considered in this study as one of the potential candidate control structures and is referred to as CS1, hereafter. Two of the most recent control structures for the HDA process, one by Konda et al. (2005) and the other by Vasbinder et al. (2004), are also considered in this study for performance assessment. Konda et al. (2005) proposed a PWC structure for the HDA process based on an integrated framework consisting of improved heuristic method and rigorous simulation tools. Vasbinder et al. (2004) proposed a PWC structure for the HDA process using decision-based approach. The former is referred to as CS2 and the latter as CS3 hereafter. Incidentally, these are the only three control structures which have made use of rigorous dynamic simulation either in the control system design stage (e.g., CS2) or in the validation stage of the resulting control system (CS1 & CS3) for the detailed HDA process.

Other notable control structures for the HDA process are by Ponton and Laing (1993) and Fonyo (1994). Konda et al. (2005) discussed the limitations of these control structures; hence, these are not considered in the present study. Other researchers have considered a simplified HDA process for control structure design (e.g., Qiu et al., 2003) while others assumed some of the control decisions are already in place (e.g., Jorgensen and Jorgensen, 2000; Herrmann et al., 2003); thus the complete PWC structure for the entire HDA process cannot directly be extracted from these works unless these methods are re-applied to develop complete PWC system. Hence, these control structures could not be considered in this study.

5.4.1 Three Selected Control Structures (CS1, CS2, CS3)

CS1 is solely based on the heuristic procedure (Luyben et al., 1999). One of the characteristic features of this heuristic procedure is to fix a flow in the recycle loop to avoid the notorious effect of recycles - snowball effect. However, as observed by other researchers, it is not always recommendable to fix the flow. For example, Zheng et al. (1999) have studied several control structures (for a hypothetical process) including the one with fixed-recycle-flow and observed that this control structure is inferior to some other structures in which the recycle flow is not fixed. CS2 is based on the integrated framework of heuristics and rigorous simulation (Konda et al., 2005); in this framework, systematic analysis is carried out on recycles while designing the control systems to minimize their impact on overall control performance. CS3 is based on decision-based methodology (Vasbinder et al. 2004) in which the modified analytical hierarchical process (mAHP) method is used to decompose the HDA process into several modules and then Luyben's heuristic procedure is applied to each module to develop PWC system.

Interestingly, though each of these methods made use of Luyben's heuristic procedure in some form or other, the resulting control systems are significantly different. Equally interesting is that these control structures can be classified into three distinctly different categories based on the TPM: CS1 uses internal variable, either reactor temperature, $T_{R\text{-}in}$ or total toluene flow, F_R (i.e., sum of fresh toluene and recycled toluene) - the present study considered both the alternatives; CS2 uses process feed (i.e., fixed-feed control strategy); and CS3 uses production rate (i.e., on-demand control strategy) as the TPM. Consequently, rest of the control structure of CS1, CS2 and CS3 are also very different, as shown in Table 5.1. CS1 and CS3 are shown in Table 5.1 after the implementation of the modifications discussed below.

The only modification that is required for CS1 is replacing the cascade controller for product purity (which manipulates the set point of temperature controller) by a controller which directly manipulates reflux to regulate product purity. This modification is observed to be necessary as the impact of the disturbance on the process and settling time is found to be less after implementing this modification. While this minor modification for CS1 is just to improve the dynamic performance, CS3 required several changes mainly to stabilize the process and also to make it more realistic. For example, Vasbinder et al. (2004) controlled H_2 to toluene ratio whereas the actual constraint for the HDA process is on the ratio between H_2 and aromatics (McKetta, 1977; Douglas, 1988). So, in the present study, H_2 to aromatics ratio controller is implemented.

With this H_2 to aromatics ratio controller, we tried to implement CS3 as was proposed by Vasbinder et al. (2004). However, the process was not stable and we have identified that there was no controller which propagates the production rate changes back to the upstream of stabilizer. Since there should be consistent back-propagation of changes in any on-demand control strategy, we have considered the stabilizer feed flow (instead of reboiler duty) as the manipulator to control stabilizer reboiler level; note that the stabilizer feed flow was used to control flash level by Vasbinder et al. (2004). The flash level is then controlled by toluene feed flow. With these changes, there is back propagation of changes and the system is stable in the presence of any common disturbance (e.g., -5% change in the throughput), however, the system becomes unstable and not able to reach steady-state for bigger disturbances (e.g., -25% change in the throughput).

After careful investigation, it was identified that the main problem is associated with the stabilizer with its over-head section getting accumulated with benzene. This can be qualitatively explained: when there is any decrease in the production rate, there will be corresponding decrease in the product column feed (i.e., stabilizer bottoms). Ideally, this change should then be reflected back; i.e., the stabilizer reboiler level increases and thus the stabilizer feed should be reduced which in turn increases the flash level, and eventually the fresh toluene feed will have to be reduced to maintain the flash level. However, due to the slow dynamics observed with on-demand control strategy, before the stabilizer feed gets reduced, the effect on the stabilizer bottoms (due to the reduction in the production rate) is felt on the stabilizer over-head section; i.e., the additional benzene and toluene, that were pushed back to the stabilizer bottoms, are observed to be entering into the stabilizer over-head section. This could be due to two reasons: (1) stabilizer has fewer trays (i.e., 10 trays) and the changes in the bottom section can easily effect the over-head section; and (2) neither the stabilizer over-head section is strong enough to counteract this (e.g., reflux flow is as low as 0.24 kg-mol/hr and thus not able to handle big changes) nor there is a bottoms composition controller to holdback any changes in the bottom section of the stabilizer. This reasoning can be substantiated based on the fact that the system reaches stable steady-state after installing a bottoms composition (i.e., inferential) controller even in the presence of production rate disturbances. In order to cross-validate the implementation, we have contacted the proponents of CS3 for their HYSYS models, but, unfortunately, the models are not available. Thus, we implemented the on-demand control strategy with the minimal modifications as discussed above. These changes are required in order to establish a stable system which can handle some common disturbances. As will be discussed in the later sections, CS3 failed to stabilize the process for six out of fifteen disturbances studied; though the process can be stabilized for the rest of the disturbances, the performance of CS3 is observed to be inferior to that of other control structures.

5.4.2 Plant-Wide Controller Tuning

Controller tuning from plant-wide perspective is tedious due to the large of number of controllers which are interacting with one another. In addition, one particular set of tuning parameters for a control system does not necessarily work for all disturbances as the impact of different disturbances on various sections of the plant can be very different. For example, by using auto-tuning technique, a controller gain of 2.3 is obtained for reactor outlet temperature controller (i.e., second controller in Table 5.2) for CS2. Though this is acceptable for most of the disturbances, the process becomes unstable for disturbances associated with uncertainty in kinetics. The tuning parameters are observed to be more aggressive for this disturbance; ten-folded reduction in the gain (i.e., a controller gain of 0.25) makes it stable for all types of disturbances. This example shows how critical the tuning parameters of each controller in the plant since inappropriate tuning parameters of single controller can make the entire process unstable. So, extensive simulations are carried out in the present study to make sure that the tuning parameters of all the controllers are robust (to give stable response for most of the disturbances) as well as aggressive enough (to give reasonably good performance). On the other hand, the same controller (which required a gain of 0.25 in CS2, i.e., second controller in Table 5.2) can be very aggressive with a gain of 1.32 in CS1 (i.e., five-times that of what is used in CS2). This explains how dependent the tuning of each controller on the overall control structure. Thus, it is important to consider the plant-wide perspective, not only during structural decisions stage but also while tuning the controllers.

In general, all the controllers (except level controllers) are designed as PI-controllers and P-only controllers are used for level control. Generic tuning parameters are given for flow, level and pressure controllers in Luyben (2002), and are used as initial estimates for these three types of controllers in all the control structures. Wherever possible, for level and pressure controllers, aggressive tuning is used (e.g., a gain of 10 for fifth controller in Table 5.2) and, if required, conservative tuning is used (e.g., a gain of 2 for several level controllers in the separation section). For temperature and composition controllers, initial estimates for tuning parameters are obtained using auto-tuning technique. Understandably, auto-tuner gives comparable tuning parameters with slight differences, if the control structure of any controller remains the same in CS1, CS2 and CS3 (e.g., 1st, 3rd, 23rd, 24th, 28th and 30th controllers in Table 5.2). The slight differences are due to the different interactions that these controllers encounter from other controllers in CS1, CS2 and CS3. Understandably, auto-tuner gave entirely different tuning parameters if the control structure of any controller is different in CS1, CS2 and CS3 (e.g., 8th controller in Table 5.2). All these controllers are then fine tuned to give stable and reasonably good performance in the presence of most of the anticipated disturbances. Final tuning parameters for the controllers in the three control structures are given in Table 5.2.

Table 5.1: Details of Controlled and Manipulated Variables of CS1, CS2 and CS3

Controlled Variable (CV)	Manipulated Variable (MV)		
	CS1#	**CS2**	**CS3#**
1. Cooler T_{out}	Cooling Water Flow	Cooling Water Flow	Cooling Water Flow
2. Reactor T_{out}	Quench Flow Rate	Quench Flow Rate	Quench Flow Rate
3. Reactor T_{in}	Furnace Fuel	-	Furnace Fuel
4. Conversion	-	Furnace Fuel	-
5. Flash Level	Stabilizer Feed	Stabilizer Feed	*Toluene Feed Flow* (Stabilizer Feed Flow)
6. Flash Pressure	-	Flash Vapor Flow	Flash Vapor Flow
7. Recycle Gas Pressure	H_2 Feed Flow	-	-
8. Purge Composition	Purge Flow	Compressor Duty	-
9. Purge Flow	-	-	Purge Flow
10. H_2 to Aromatics Ratio	-	H_2 Feed Flow	H_2 Feed Flow
11. Total Toluene Flow	Total Toluene Flow	-	-
12. Toluene Feed	-	Toluene Feed Flow	-
Stabilizer			
13. Condenser Pressure	Distillate Flow	Distillate Flow	Distillate Flow
14. Condenser Level	Condenser Duty	Condenser Duty	Condenser Duty
15. Reboiler Level	Bottoms Flow	Bottoms Flow	*Stabilizer Feed Flow* (Reboiler Duty)
16. Distillate Composition	-	Reflux Flow	Reflux Flow
17. Reflux Flow	Reflux Flow	-	-
18. 7^{th} Tray Temperature*	Reboiler Duty	Reboiler Duty	*Reboiler Duty* (no manipulator)
Product (Benzene) Column			
19. Condenser Pressure	Condenser Duty	Condenser Duty	Condenser Duty
20. Condenser Level	Distillate Flow	Distillate Flow	Product Column Feed
21. Reboiler Level	Bottoms Flow	Bottoms Flow	Bottoms Flow
22. Product (Benzene) Flow	-	-	Distillate Flow
23. Distillate Composition	*Reflux Flow* (set point of bottoms temperature controller)	Reflux Flow	Reflux Flow
24. 40^{th} Tray Temperature*	Reboiler Duty	Reboiler Duty	Reboiler Duty
Recycle (Toluene) Column			
25. Condenser Pressure	Condenser Duty	Condenser Duty	Condenser Duty
26. Condenser Level	Toluene Feed Flow	Distillate Flow	Distillate Flow
27. Reboiler Level	Reboiler Duty	Reboiler Duty	Bottoms Flow
28. Distillate Composition	-	Reflux Flow	Reflux Flow
29. Reflux Flow	Reflux Flow	-	-
30. Bottoms Composition	-	Bottoms Flow	Reboiler Duty
31. 18^{th} Tray Temperature*	Bottoms Flow	-	-

*Trays are counted from the top, with condenser as 0^{th} tray.

#CS1 and CS3 are shown in this table after the implementation of the modifications, as per the discussion in Section 5.4. Modified MVs are italicized and the original MVs are bracketed.

5.4.3 Disturbances Studied

It is very common to consider two or three types of disturbances while assessing the performance of control systems. However, as will be discussed in section 5.5, the control structure that works for a disturbance does not necessarily work for other types of disturbances as the nature of each disturbance is unique. Thus, there is a need to study several anticipated disturbances. Hence, in the present study, 15 important and most common disturbances are studied (Table 5.3). As there is a possibility of encountering more than one disturbance at a time, we have considered dual disturbances as well. For example, the disturbances d_8 to d_{11} are essentially the combinations of other disturbances (i.e., d_1 and d_2 with d_4 and d_5; any other combination can also be considered). Similarly, uncertainties in reaction kinetics are also simulated as disturbances. For convenience, a tag is assigned to each disturbance; i.e., first disturbance will be referred to as $d_{1,}$ second one as d_2 and so on (see Table 5.3).

Table 5.2: Tuning Parameters for the Controllers in CS1, CS2 and CS3

Controller Name	Tuning Parameters K_c (%/%), T_i (Min)		
	CS1	CS2	CS3
1. Cooler T_{out} Controller	0.13, 0.14	0.15, 0.29	0.15, 0.29
2. Reactor T_{out} Controller	1.32, 0.24	0.25, 0.25	2.3, 0.27
3. Reactor T_{in} Controller	0.14, 0.22	-	0.14, 0.22
4. Conversion Controller	-	1, 2	-
5. Flash Level Controller	10	10	10
6. Flash Pressure Controller	-	2, 5	2, 2
7. Recycle Gas Pressure Controller	1.73, 2.17	-	-
8. Purge Composition Controller	1.19, 23.2	4.94, 4.02	-
9. Purge Flow Controller	-	-	0.5, 0.25
10. H_2 to Aromatics Ratio Controller	-	0.5, 0.25	0.5, 0.25
11. Total Toluene Flow Controller	0.5, 0.25	-	-
12. Toluene Feed Controller		0.5, 0.25	
Stabilizer			
13. Condenser Pressure Controller	2, 10	2, 10	2, 25
14. Condenser Level Controller	2	5	2
15. Reboiler Level Controller	5	2	2
16. Distillate Composition Controller	-	0.1, 10	0.12, 10
17. Reflux Flow Controller	Flow specified	-	-
18. 7^{th} Tray Temperature Controller	10, 7.02	10, 5.54	10, 5.62
Product (Benzene) Column			
19. Condenser Pressure Controller	2, 10	2, 10	2, 25
20. Condenser Level Controller	5	2	2
21. Reboiler Level Controller	5	2	2
22. Product (Benzene) Flow Controller	-	-	0.5, 0.25
23. Distillate Composition Controller	0.84, 13.3	0.65, 13	1.34, 8.61
24. 40^{th} Tray Temperature Controller	8.5, 1.07	7.44, 0.85	6.48, 1.04
Recycle (Toluene) Column			
25. Condenser Pressure Controller	2, 25	2, 20	2, 25
26. Condenser Level Controller	5	5	2
27. Reboiler Level Controller	2	5	5
28. Distillate Composition Controller	-	0.14, 49.8	0.14, 39.5
29. Reflux Flow Controller	Flow specified	-	-
30. Bottoms Composition Controller	-	0.15, 38	0.11, 35.9
31. 18^{th} Tray Temperature Controller	0.2, 50	-	-

5.5 Results and Discussion

The three control structures, CS1, CS2 and CS3, are evaluated for 15 disturbances, and their performance in terms of DDS is given for all the disturbances (Table 5.3). As discussed above, the lesser the DDS, the better is the control system. In general, different disturbances have different impact on the process; for example, the effect of d_{14} and d_{15} on the process is very much less when compared to the impact of other disturbances. Also, the performance of control systems differs significantly, as discussed below in detail. The only control structure that can stabilize the process in the presence any of the disturbances studied is CS2 with performance that is either superior or comparable to that of CS1 and CS3 (Table 5.3). In the following sections, the performance of all the three control structures is evaluated with regard to DDS, and is observed that CS2 is superior. The analysis based on process and equipment constraints, robustness and stability concerns also leads to the same conclusion that CS2 does a better job and, thus, further justifying the use of DDS as PWC performance metric.

In general, rigorous nonlinear dynamic simulation is observed to be very challenging due to the varying valve pressure-drop requirements of each control structure; for example, valve on purge stream in CS3 reached saturation limits for d_1 when it is sized for a reasonable pressure drop of 50 psi and required larger pressure drop of 200 psi. On the other hand, in CS1 and CS2, purge valve, with a pressure drop of 50 psi, was not saturated for the same disturbance. To make the situation worse, the pressure-drop requirements for any control structure are even dependent on the type of disturbance; for example, the purge valve, with a pressure drop of 50 psi, was not saturated for any change in toluene feed temperature (i.e., d_{14} and d_{15}) whereas, as mentioned above, it is saturated for the throughput changes. In addition, all these issues are very much dependent on pump characteristics. These are some of the important aspects during any PWC structure analysis as the selection of control structure has large impact on pressure-drop requirements which in turn affects plant economics. Despite their importance, these issues have not been given enough importance in the earlier PWC studies as most of them are based on simplified models (e.g., ignoring the pump characteristics and valve dynamics) which simplifies the analysis but at the cost of realistic behavior of the process. This issue is discussed in detail in the later part of this section.

Table 5.3: Disturbances Studied and Corresponding DDS for Control Structures: CS1, CS2 and CS3

	Type and magnitude of disturbance		DDS (kg-mol)		
			CS1	CS2	CS3
d_1	Production rate	-5%	10.41 (F_R) 20.05 ($T_{R\text{-}in}$)	8.70	78.75
d_2		+5%	9.68 (F_R) 19.67 ($T_{R\text{-}in}$)	8.68	Unstable
d_3		-25%	41.45 (F_R) Unstable ($T_{R\text{-}in}$)	47.93	Valve Saturation
d_4	Feed Composition	-2.5%	5.34	1.92	Unstable
d_5		+2.5 %	4.92	1.78	68.14
d_6	Uncertainty in Kinetics (Pre-Exponential factor of first reaction)	+5%	13.59	13.62	31.73
d_7		-5%	15.14	17.29	Unstable
d_8	Dual Disturbances	d_1 & d_5	12.71 (F_R) 20.84 ($T_{R\text{-}in}$)	9.26	144.38
d_9		d_1 & d_4	9.61 (F_R) 19.61 ($T_{R\text{-}in}$)	9.14	41.29
d_{10}		d_2 & d_5	8.47 (F_R) 20.62 ($T_{R\text{-}in}$)	9.07	Unstable
d_{11}		d_2 & d_4	12.45 (F_R) 19.09 ($T_{R\text{-}in}$)	9.08	Unstable
d_{12}	H2 Header Pressure	+5%	6.54	2.58	2.60
d_{13}		-5%	10.37	5.83	5.82
d_{14}	Toluene Feed Temperature	+10^0 C	0.74	0.63	0.72
d_{15}		-10^{0}C	0.67	0.58	0.69

5.5.1 Evaluation of CS1 and CS2

CS1 has two potential TPMs: 1) F_R, and 2) $T_{R\text{-}in}$. Thus, both the TPMs are considered in this study, and represented as F_R and $T_{R\text{-}in}$ in Tables 5.3 to 5.7 based on what manipulator is used to achieve the throughput changes. It is of interest to see which one is the better manipulator for CS1. In general, the dynamic behavior of the process, especially, separation section (i.e., three distillation columns), is very different for both these TPMs. The changes in vapor flow rate within the three distillation columns for ±5% change in the throughput (using both the manipulators) are given in Table 5.4. It can be seen that, with $T_{R\text{-}in}$ as the TPM, recycle column is much more sensitive than the other two columns; change in internal-vapor flow rate of recycle column is +12.77% compared to -2.85% and +0.58% changes in product and stabilizer columns respectively. Thus, the robustness of CS1 with $T_{R\text{-}in}$ as the manipulator largely depends on recycle column. On the other hand, with F_R as the TPM, recycle column becomes relatively less sensitive compared to other columns (-1% change in internal vapor flows of recycle column vs -4.67% and -3.72% changes in product column and stabilizer respectively for -5% change in the throughput). In this case, though the impact of the disturbances is transferred to the other columns (which eventually made product and stabilizer columns relatively more sensitive to disturbances), none of the columns is as severely affected as the recycle column in the process with CS1 and $T_{R\text{-}in}$ as the TPM. Thus, with F_R as the TPM, CS1 is more robust and handles bigger disturbances.

It can now be concluded that fixing a flow in order to avoid snowball effect, though a feasible alternative, does not serve the purpose if the TPM is not chosen appropriately; else, it will only transfer the snowball effect from one part of the process to another (i.e., from total toluene flow to recycle column in this case). Similar observation is made by Yu (1999) in case of a simple reactor-separation-recycle network. On the other hand, with CS2, the effect of disturbances on all three distillation columns is almost comparable thus making CS2 a balanced control structure (Table 5.4). The presence of conversion controller is the main reason for this balanced nature of CS2 (Konda et al., 2005).

With $T_{R\text{-}in}$ as the TPM, in the presence of -5% change in the production rate, as shown in Table 5.4, variation in the vapor loads of the recycle column is much higher than that of the product and the stabilizer columns (i.e., +12.77% versus -2.85% and +0.58%). Moreover, the vapor loads in the product column decreased whereas the vapor loads in the recycle column and the stabilizer increased (Table 5.4). Consequently, there is a significant increase in the steam requirement for the recycle column's reboiler (Table 5.5). On the other hand, CS2 and CS1 with F_R as the TPM exhibited relatively more uniform dynamics by almost equally distributing the impact of the disturbance amongst all the columns (Tables 5.4 and 5.5). Further, variation in the steam requirement for the recycle column's reboiler is much less (Table 5.5). Similarly, changes in the internal liquid flows in the columns are highly non-uniform if the $T_{R\text{-}in}$ is the TPM for CS1; for example, for $\pm$5% changes in the throughput, the changes in internal liquid flows of different trays of toluene column are very much different, with a minimum and maximum change of -6% and +12% respectively. On the other hand, for CS1 with F_R as the TPM, the changes are quite uniform with a minimum and maximum change of 10% and 13% respectively, thereby exhibiting more linear (internal) column dynamics, and thus a linear controller (such as a PID type controller) performs better.

Table 5.4: Percentage Change* in the Net Vapor Flow of Three Columns in the Presence of Disturbances for CS1 and CS2

	-5% change in throughput			+5% change in throughput		
	CS1 with TPM as		CS2	CS1 with TPM as		CS2
	$T_{R\text{-}in}$	F_R		$T_{R\text{-}in}$	F_R	
Recycle Column	+12.77	-1.0	-5.17	-12.94	+0.62	+5.17
Product Column	-2.85	-4.67	-5.17	+2.65	+4.58	+5.18
Stabilizer	+0.58	-3.72	-5.08	-0.58	+3.67	+5.09

*Values given are the average over all trays; as the variation in the % deviation of vapor flows is very less, average value is a good indication of the change on every tray

Table 5.5: Percentage Change in Reboiler Duties of Three Distillation Columns in the Presence of -5% Throughput Change for CS1 and CS2

	-5% change in throughput		
	CS1 with TPM as		CS2
	$T_{R\text{-}in}$	F_R	
Recycle Column	+11.0	-3.7	-5.2
Product Column	-2.96	-4.7	-5.2
Stabilizer	+1.6	-1.4	-5.2

Furthermore, with $T_{R\text{-}in}$ as the TPM the process exhibits inverse response for the throughput changes; but this is not the case when F_R is used as the TPM although the response is more complex (Figure 5.4). Figure 5.4 shows the production rate transients with both the manipulators to achieve -5% change in the throughput (Figure 5.4, left); the impact of inverse response is more for bigger changes in the throughput (Figure 5.4, right).

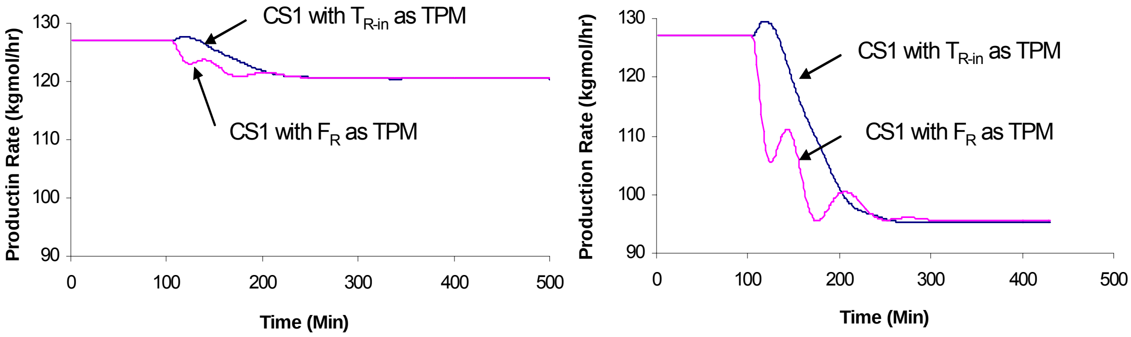


Figure 5.4: Production Rate Variation for CS1 to Achieve -5% (left) and -25% (right) Changes in the Throughput

Equipment Constraints: Based on the above discussion, it now logically follows that the probability of hitting constraints in the presence of disturbances is high if $T_{R\text{-}in}$ is the TPM. For example, operational constraints related to 'dry-hole pressure drop (ΔP_{dry})' of recycle column are found to be violated in the presence of several disturbances, i.e., ΔP_{dry} exceeds maximum allowable ΔP_{dry} (Table 5.6). Note that, for any change in the throughput (i.e., d_2, d_{10} and d_{11}), the ΔP_{dry} constraints are violated even for CS2; however, the violation in this case is less severe (Table 5.6).

Table 5.6: Dry Hole Pressure Drop for the Recycle Column in CS1 and CS2

Maximum allowable ΔP_{dry} for CS1 and CS2 for the base-case HDA process (i.e., without any disturbance)	2.57 psi
Calculated ΔP_{dry} for CS1 in the presence of d_1, d_2, d_3, d_8 and d_9 with $T_{R\text{-}in}$ as the TPM*	3.04 psi
Calculated ΔP_{dry} for CS2 in the presence of d_2, d_{10} and d_{11} with F_R as the TPM*	2.60 psi

*Calculated ΔP_{dry} is within the maximum allowable value for other disturbances

Also, in the presence of disturbances, proper functioning of CS1 needed flat head characteristics (i.e., head as the pump dynamic specification) for the recycle toluene and fresh toluene feed pumps. Else, with rising head characteristics (i.e., duty as the specification – with this specification, head developed by the pump decreases as the flow increases), very large pressure drops are required for the valves in recycle section to handle disturbances. For example, with flat head characteristics for these pumps, CS1 is able to achieve -5% change in the throughput, using either F_R or $T_{R\text{-}in}$ as the TPM, with a reasonable pressure drop of 20-50 psi across all the valves in the process. However, with rising head characteristic, some valves in recycle section needed larger pressure drops (e.g., valve on total toluene flow needed as large pressure drop as 200 psi) to achieve -5% change in the throughput using $T_{R\text{-}in}$ as the TPM, though it could be achieved with a reasonably smaller pressure drop if F_R is used as the TPM. In general, it is observed that, for rising head characteristics for the pumps in recycle section, valve pressure drops required to achieve any amount of throughput change are larger if $T_{R\text{-}in}$ is used as the TPM than those required if F_R is the TPM. On the contrary, in case of CS2, the process is able to achieve the throughput changes with reasonable pressure drops (i.e., 20–50 psi) irrespective of characteristics of pumps in the recycle section.

In general, single-stage high-speed centrifugal pumps are recommended for the pumps in recycle- and toluene-feed sections, based on operating conditions, i.e., low-flow, high head requirements and low-viscosity fluids (Woods, 1995). Such pumps can exhibit either flat or rising head characteristics (McGuire, 1990). However, CS1 requires flat head characteristics for these pumps; On the other hand, CS2 exhibited comparable performances for both types of pump characteristics, which means that CS1 puts more restrictions on design considerations. For a fairer comparison with reasonable pressure drops across valves, flat head characteristic is chosen (i.e., head is specified in the dynamic simulation) for the pumps in the recycle section. This discussion demonstrates that, also as pointed by Davidson and Bertele (2000), at times, the control structure has an effect on the choice of pump, thereby highlighting the dynamic implications of steady-state design aspects.

Operational Constraints: There is no explicit control over H_2 to aromatics ratio in CS1, and, the ratio is observed to be varying between 4.8 and 6 depending on the disturbance. In contrast, the regulation of this ratio in CS2 is better and controlled at 5 in the presence of all disturbances. This is an important constraint for the HDA process as it has both economical and operational implications. In order to avoid coking, it is recommended to keep the ratio more than 5. However, from economic perspective, it is good to keep it as low as possible. Hence, an intuitive compromise between economics and operations is to keep it as close as possible to 5.

Though there is no direct control over reactor pressure in CS2, variation in the reactor pressure in the presence of all the expected disturbances is observed to be not significant. For example, in the presence of the worst case disturbance (-25% variation in the throughput, i.e., d_3 in Table 5.3), around 2% change in the reactor pressure is observed (i.e., a deviation of 11.3 psia from 500 psia). For the rest of the disturbances, the change in reactor pressure is much less (< 1%). Also, any negative effect due to the pressure change is somewhat compensated by the conversion controller which ultimately varies the reactor temperature to maintain the conversion and thereby regulating the throughput. Thus, an explicit control action over reactor pressure is not needed if CS2 is chosen as the control structure.

Robustness and Stability: Though CS1 is able to stabilize the process for most of the disturbances, it is not able to handle large changes in the throughput using the reactor temperature ($T_{R\text{-}in}$) as the TPM (Table 5.3). Even -15% change in the throughput could not be achieved using $T_{R\text{-}in}$ as the TPM as the process becomes unstable (Figure 5.5). Though the stability can be achieved for other disturbances, the performance is not as good as what can be achieved using F_R as the TPM. For example, in the presence of disturbance d_1, DDS for CS1 with F_R as the TPM (10.41) is nearly of that of CS1 with $T_{R\text{-}in}$ as the TPM (20.05). Even -25% change in the throughput (d_3 in Table 5.3) can be accomplished by making use of F_R as the TPM (Figure 5.5). In general, CS1 with $T_{R\text{-}in}$ as the TPM is more sensitive in comparison to CS1 with F_R as the TPM (this is also reflected from larger values of DDS for CS1 with $T_{R\text{-}in}$ as the TPM given in Table 5.3) and is less robust. This observation contradicts the conclusion made by Luyben et al. (1999) who observed that larger changes in the throughput can be accomplished using $T_{R\text{-}in}$ as the TPM. This could be due to several reasons: (1) Luyben et al. (1999) assumed ideal vapor-liquid equilibrium (VLE), whereas, the present study uses the Peng-Robinson (PR) equation of state to predict VLE behavior; we have observed that the choice of property package can significantly affect the column conditions. For example, with ideal VLE assumption, a maximum of 9%, 21% and 22% variation (compared to the values obtained using PR equation of state) is observed in tray temperature, net liquid and net vapor flows, respectively. (2) simplified models for some units are used in the study by Luyben et al. (1999), e.g., stabilizer is modeled as a splitter and tank compared to realistic simulation as a column in the present study, and (3) the differences in the simulation programs; Luyben et al. (1999) used TMODS dynamic simulator, while this study is based on HYSYS.

Performance: Though CS1 with F_R as the TPM is able to handle all the disturbances, the performance, especially with respect to the recycle column, is slightly inferior to that of CS2 (Figure 5.6). CS2 is able to regulate the temperature within the sensor range while the temperature in CS1 crosses the sensor limits; note that, though the biphenyl concentration, but not the tray temperature, is controlled in CS2, tray temperature profile of CS2 is shown in Figure 5.5 for the sake of comparison). For several other disturbances, CS1 with F_R as the TPM exhibited comparable performance with CS2. Its performance in the presence of feed composition and H_2 pressure disturbances (i.e., d_4, d_5, d_{12} and d_{13}) is, however, relatively poor. In addition, one of the merits of CS2 is that it gives stable performance for all the anticipated disturbances.

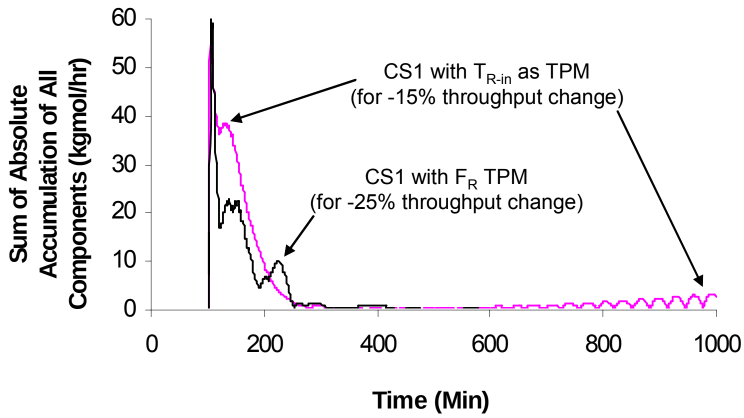


Figure 5.5: Accumulation Profile for the Process with CS1 for a Throughput Change

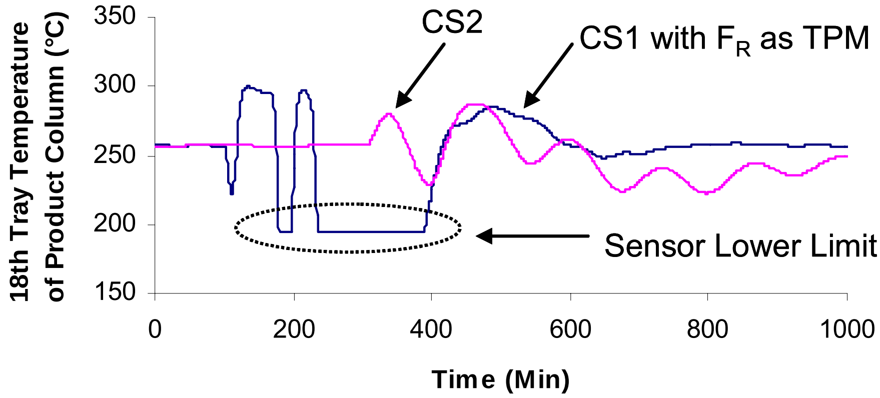


Figure 5.6: Recycle Column Tray Temperature Transient for -25% Throughput Change

5.5.2 Evaluation of CS3

CS3 failed to stabilize the process in the presence of nearly half of the disturbances (i.e., d_2, d_3, d_4, d_7, d_{10}, d_{11}); though, for some disturbances (i.e., d_1, d_5, d_6, d_8 and d_9), CS3 is able to stabilize the process, performance is observed to be poor. For example, in the presence of d_1, DDS for CS2 is only 11% of that of CS3 (Table 5.3). In general, CS3 is observed to be relatively more sensitive to disturbances (as can be interpreted from the large values of DDS of CS3 in Table

5.3) and thus, it is less robust (i.e., CS3 cannot handle large disturbances). For example, even for -10% change in the throughput, some control valves operate close to constraints, i.e., valve opening is less than 10% (Figure 5.7). So, valves reach saturation limits for bigger disturbances (e.g., d_3 in Table 5.3, i.e., -25% change in the throughput). Similarly, even for a small increase (e.g., +1%) in the throughput, the process is significantly affected and hence, for +5% change in the throughput (i.e., d_2 in Table 5.3), the process becomes unstable (Figure 5.8). For the process with CS3, due to the instability in the presence of d_2, the product quality became uncontrollable and reached lower sensor limit at about 900 min; and the corresponding manipulated variable saturated with 100% valve opening (Figure 5.8, top). The production rate also cannot be regulated at the desired set-point (Figure 5.8; bottom). Considering these results, it appears that plant-wide perspective is not preserved in CS3. However, it is interesting to note that the performance of CS3 is comparable to that of CS2 and CS1 for disturbances d_{14} and d_{15}, and it is better than that of CS1 for disturbances d_{12} and d_{13} (Table 5.3).

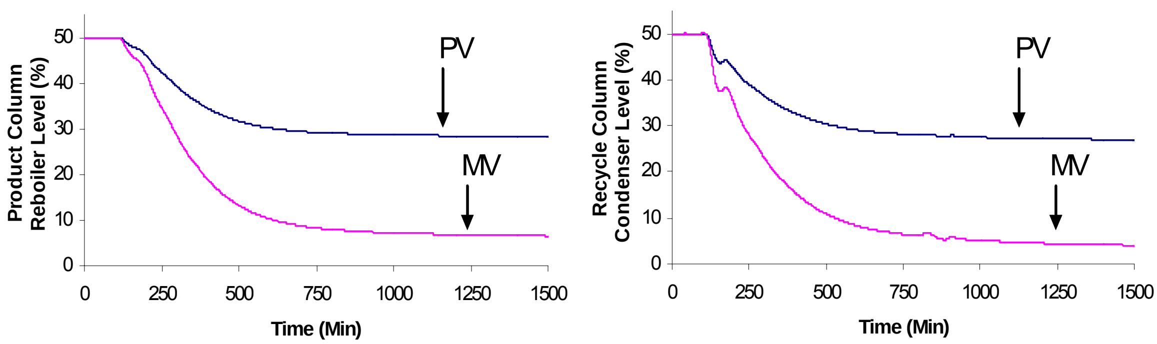


Figure 5.7: Response of Some Variables for the Process with CS3 for a -10% Change in the Throughput

To conclude, for all the disturbance scenarios, no control structure can give better performance than any other control structure. Hence, it is more appropriate to choose the control structure that gives either reasonably comparable or better performance for most, if not all, of the disturbances. For the HDA process, the performance of CS2 is either superior or comparable to that of CS1 and CS3, and thus, recommended as the final control structure. In general, recycle column, out of all the equipments, is observed to be the most sensitive with any of the control structures and is the root-cause of instability. For example, for large changes in the throughput, CS1 is observed to be unstable mainly due to the failure of recycle column. Thus, the modified HDA process without recycle column (i.e., the process in which biphenyl is being recycled) may be a better choice from control perspective. This alternative, in addition to several others, has recently been studied by Konda et al. (2006) and, is, indeed, observed to be superior from the standpoint of control. However, Konda et al. (2006) have considered only CS2 but not CS1 and CS3. One can expect that CS1 and CS3 performs better for the modified HDA process (as there is no recycle column) than the conventional HDA process. In order to quantify this, rigorous dynamic simulations for the modified HDA process with all the control structures need to be carried out; this is beyond the scope of the present study.

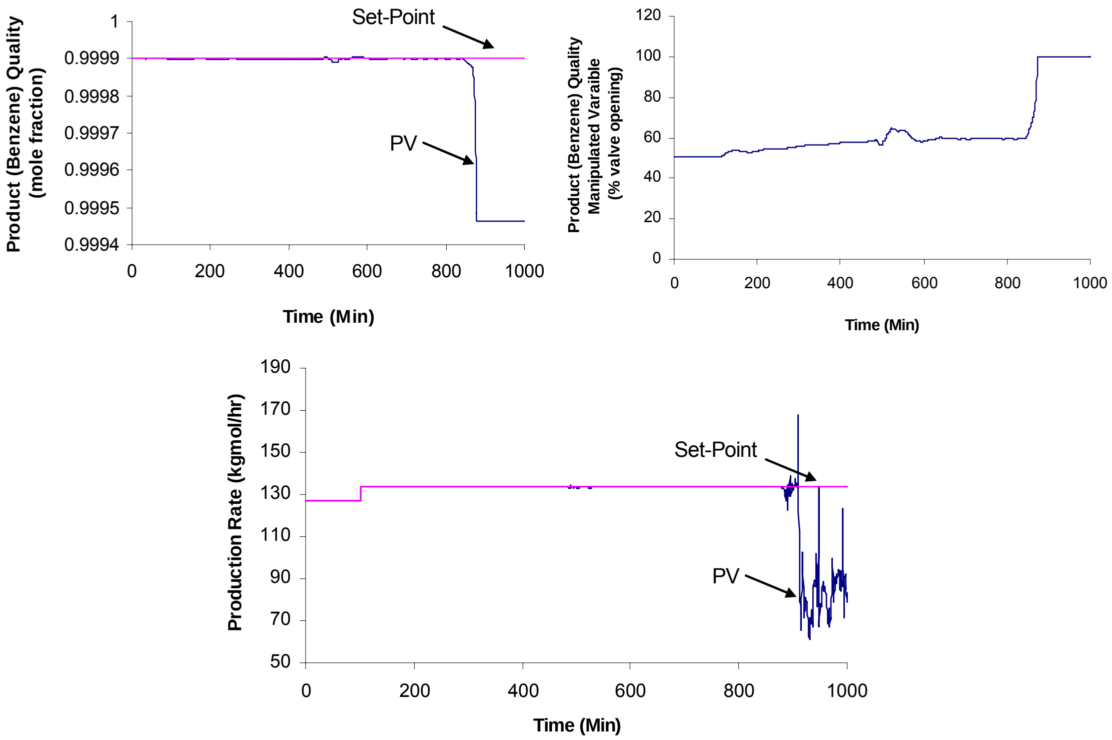


Figure 5.8: Response of Some Variables for the Process with CS3 for a +5% Change in the Throughput

5.5.3 DDS as a Troubleshooting Tool

DDS facilitates faster troubleshooting (e.g., detection of instability). For example, CS3 becomes unstable in the presence of disturbances related to uncertainty in the kinetics, which is mainly due to the inability of the recycle column's control system to mitigate the impact of disturbances. However, many other process variables (e.g., levels in the product column) appear to be reaching steady-state (Figure 5.9, top) and thus did not capture the process instability. On the other hand, accumulation profiles have captured the instability as and when it took place (Figure 5.9, bottom). What is more interesting is that, the accumulation profile for the product column (where all the process variables appear to be reaching steady-state) also captures the instability. Similarly, the accumulation profiles around other unit-operations (e.g., reactor, stabilizer and benzene column) also capture instability even though the associated process variables appear to be reaching steady-state (Figure 5.10). This emphasizes the fact that accumulation profile preserves the plant-wide perspective and thus it can be a better measure for plant-wide performance assessment. At times, depending on the severity of the accumulation and process complexity, it might take hours or even days to recognize any instability through the process variables. On the other hand, accumulation profiles (either local or plant-wide) signal instability quickly if there is instability anywhere in the plant. For example, from Figure 5.8, the process instability can be identified only after 900 min of operation. On the other hand, as shown in Figure 5.11, instability can be identified soon after 400 min of operation from accumulation profiles of the entire plant.

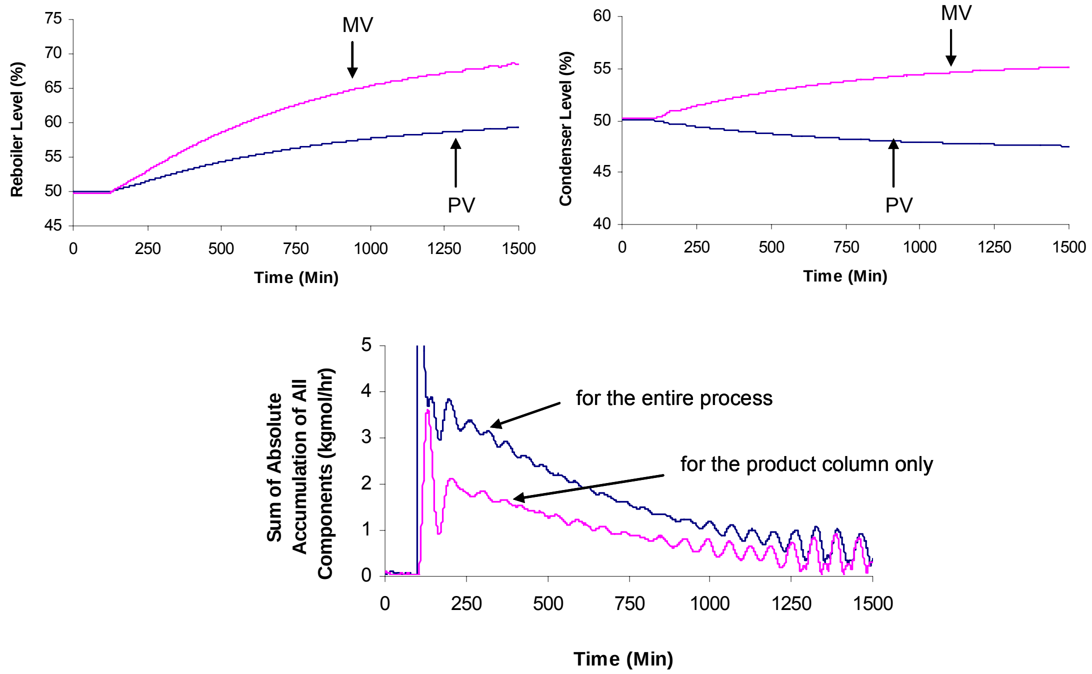


Figure 5.9: Product Column Level (above) and Accumulation (below) Profiles for the Process with CS3 in the presence of Uncertainty in the Reaction Kinetics (i.e., d_7)

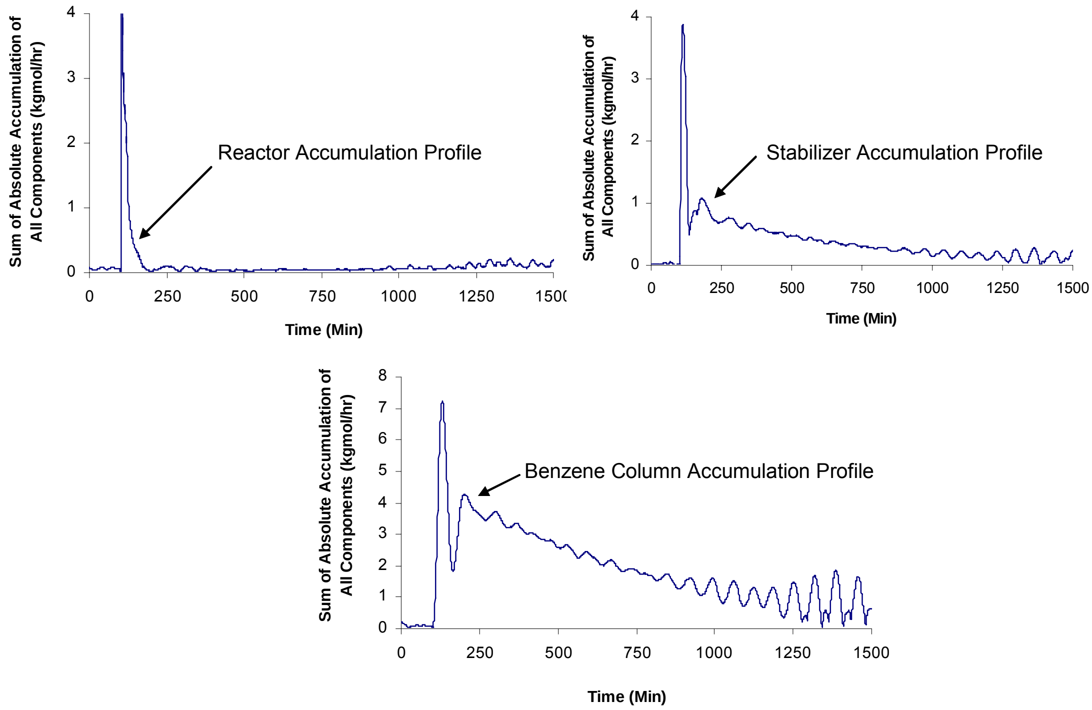


Figure 5.10: Accumulation Profiles for Different Units in the Process with CS3 in the Presence of Uncertainty in the Reaction Kinetics (i.e., d_7)

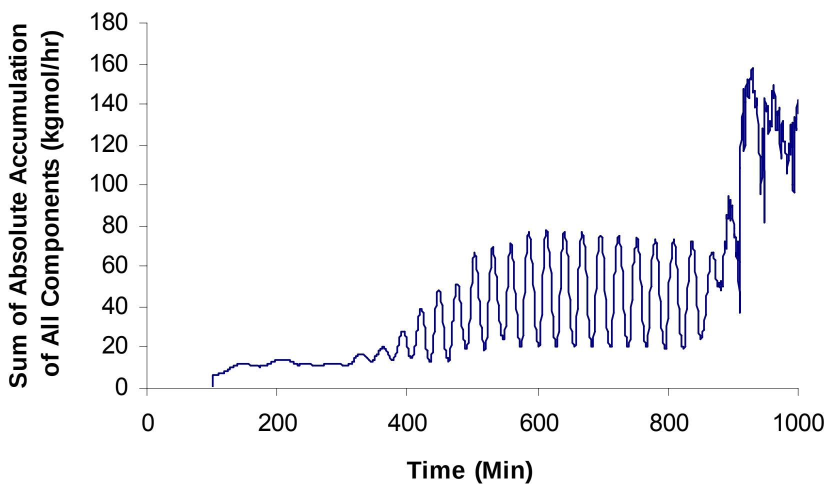


Figure 5.11: Accumulation Profile for the Process with CS3 for a Change of +5% Throughput (i.e., d_2)

5.5.4 Simplified Computation Procedure for DDS

In order to compute DDS, composition of all inlet and exit streams to the process is necessary. At times, concentration of some components may not be available. Thus, it will be useful to see how DDS will be affected if some components are ignored. Obviously, one cannot ignore the components present in large quantity, such as toluene and benzene in the HDA process. So, we ignored biphenyl, which is present in smaller quantity and recomputed DDS for the various disturbances for the process with CS1 and CS2. From Figure 5.12, it can be concluded that biphenyl can be ignored and, still, DDS can be computed with reasonable accuracy for the HDA process, thereby making it further easier to compute. DDS was also computed by ignoring methane and hydrogen along with biphenyl; and it was found that ignoring them in the HDA process is not desirable for accurate results as they are in significant quantity.

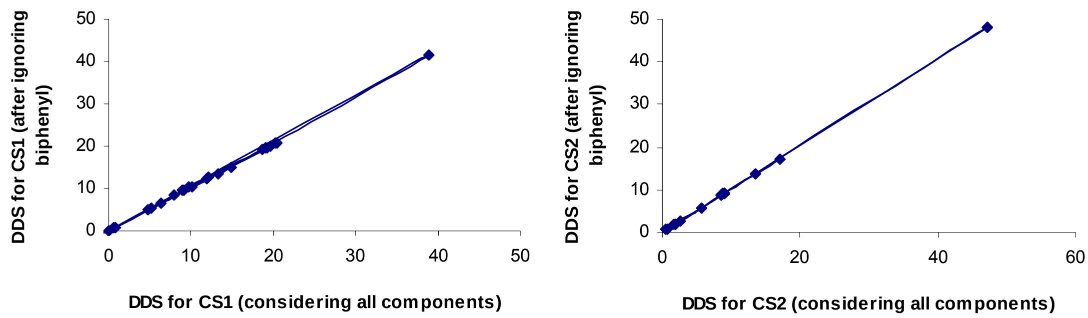


Figure 5.12: Parity Plots of Absolute Values of DDS (before and after ignoring biphenyl) for CS1 (left) and CS2 (right)

5.6 Summary

A performance metric, DDS, is proposed based on component accumulation profiles which is then successfully used to assess the performance of three PWC systems for the HDA process using rigorous nonlinear dynamic simulation. As discussed in Section 5.2, DDS has several advantages; some of them are: DDS is equally applicable to linear and nonlinear processes, computation procedure of DDS remains the same irrespective of the control structure, DDS can be computed easily using rigorous process simulators, and it facilitates early detection of instability.

From the preliminary studies, it is noted that the DDS is proportionately related to control effort (i.e., control valve movement) but further study needs to be carried out to quantify this observation. In addition, it should be noted that DDS used in this study gives equal priority to all the components and also to the positive and negative deviations. Hence, if these assumptions are not true for any process (e.g., if some components are measured at ppm level while others are not), DDS should be appropriately modified, perhaps by considering functions of accumulation of components while computing DDS. However, such a procedure can be process-specific (e.g., what should be the function?) and further investigation needs to be carried out before coming to a conclusion. Since DDS is more fundamentally defined based on the accumulation in the component material balances, it is more useful for plant-wide performance analysis. For example, the DDS values over the subsections of the plant, after normalization, are additive (in order to compute DDS over the entire process). On the other hand, IAE values are not additive as they can be defined for any process variable (e.g., temperature, pressure, composition or levels). Though, DDS do not directly capture the variation in all these process variables, it indirectly captures the impact through accumulation profiles as any change in these process variables always effects component material balances. But the normalization of DDS values over different sections of the plant, on the basis of either section inventory or flows, needs further investigation so that it can be generalized.

Dynamic performance of three PWC systems (CS1, CS2 and CS3) for the HDA process in the presence of several anticipated disturbances shows that they exhibit entirely different behavior. In general, CS2 (the balanced control structure with the fixed-feed TPM), is observed to be offering superior or comparable performance over CS1 (control structure with the internal TPM) and CS3 (on-demand control structure). In addition, satisfaction of operating constraints (such as H_2 to aromatics ratio and dry-hole pressure drops in distillation columns) in CS2 is better, and CS2 is more flexible from steady-state design standpoint (e.g., choice of pump characteristics). The performance of CS1 is found to be largely dependent on the choice of TPM. With F_R as the TPM, the performance of CS1 is comparable to that of CS2 for many disturbances; with $T_{R\text{-}in}$ as the TPM, however, the process is more sensitive to disturbances and thus less robust. CS3 exhibited very slow dynamics and is more sensitive to the disturbances; thus, it is not able to stabilize the process for most of the anticipated disturbances. Despite these advantages, the use of CS2 may be hindered as it requires more composition measurements. However, considering the advances in composition analyzer technology and its increasing industrial applications, one can foresee that it will be less of a concern

CHAPTER 6

PLANT-WIDE INTERACTION OF DESIGN AND CONTROL*

Integration of process design and control has been receiving growing interest in recent years to reap both economic and operational benefits. Thus, in this chapter, a modified sequential approach consisting of two stages and combining rigorous nonlinear simulation with heuristics is proposed for integrated design and control of industrial processes. In the first (i.e., design) stage, several alternatives are systematically generated and ranked based on economics. A few top-ranked alternatives from the design stage are then forwarded to the second (i.e., control) stage for further analysis on their dynamics to arrive at the best process that is economical as well as easy to operate. Nonlinear simulation is combined with heuristics for realistic analysis in each stage. The control system performance measure, namely, dynamic disturbance sensitivity (DDS), which was proposed in Chapter 5, is used to assess the dynamic performance of process designs and control structures. Application of the proposed approach to the HDA process is described in detail. The dynamics of the most economical process alternative are found to be inferior to those of slightly less economical alternatives, which highlight the need for plant-wide studies on the interaction of design and control.

6.1 Introduction

Design engineers try to design the most economical processes while control engineers need processes that are the best operable. However, many a times, the objectives of these two groups, design and control, may contradict. For example,

* This chapter is based on the paper - Konda, N.V.S.N.M., Rangaiah, G.P. and Lim, D.K.H. Optimal Process Design and Effective Plant-Wide Control of Industrial Processes by Simulation-based Heuristic Approach, Ind. Eng. Chem. Res., 45, pp. 5955-5970. 2006.

economically optimal processes may be difficult to control and vice versa, in which case, a compromised solution has to be developed. Hence, it is important to understand the interaction effects between design and control in order to be able to strike the right balance for overall good results (Seferlis and Georgiadis, 2004; Seider et al., 2004). Interaction between design and control in the context of single units has been studied by researchers over the last couple of decades. However, relatively fewer attempts have been made on the interaction effects between process design and PWC system design. One obvious reason for this is the inherent complexity of large-scale industrial processes. In particular, processes with recycles introduce difficulties during process design as well as control system design (Kumar and Daoutidis, 2002). Analysis would be more complicated and rigorous treatment is needed before finalizing the design. Thus, integrated design and control from the plant-wide perspective is needed, which is precisely the subject of this chapter.

Although, there have been several attempts on design and control in the recent past (Luyben, 2000b; Reyes and Luyben, 2000 & 2001; Chen and Yu, 2003; Chien et al., 2004), most of them presume that the design and/or control alternatives are somehow available. In contrast, the present work systematically generates several design alternatives and then designs effective control systems for the attractive alternatives. Several researchers studied the interaction of design and control for hypothetical processes with a given process design and control structure (Grassi, 1993; Lyman and Luyben, 1996; Wu and Yu, 1997; Luyben, 2000c & 2001; Cheng and Yu, 2003); however, their primary importance is on the effect of parametric decisions on control. Present work aims at generating several process alternatives and studying the impact of both structural and parametric decisions on control from the plant-wide perspective, using rigorous nonlinear models.

Integrated design and control approaches can be broadly classified into two categories: (1) simultaneous design and control, and (2) sequential design and control (Meeuse and Grievink, 2004). In the former approach, control aspects are considered during each stage of design. The simultaneous approaches can further be classified based on (i) controllability measures and (ii) optimization. In the former, controllability metrics are used to gauge the ease of control of a particular process design. However, most often, this analysis is performed using either steady-state or linear dynamic models, which usually introduces significant approximations and, hence might not be able to characterize dynamic behavior of plants with sufficient accuracy (Sakizlis et al., 2004). The optimization-based methods have been successfully applied to simple problems involving a small number of units (Luyben and Floudas, 1994; Perkins and Walsh, 1996; Kookos and Perkins, 2001b). However, their application to large-scale plants becomes cumbersome, because of the large combinatorial explosion of alternatives. Moreover, using simultaneous methods, it is not always possible to take the best possible control decision during the initial stages of design, because of the lack of sufficient information. Hence, these decisions, which were taken in the early stages, may have to be revised in the later stages. In addition, as the best alternative would not surface until the designer explores the entire search space, typically, every process alternative would have to be considered in both the design and control stages. This can be extremely time-consuming, especially in the context of PWC, because economically unattractive alternatives would also be studied from control viewpoint.

In the sequential approach, design and control are performed sequentially (e.g., Alhammadi and Romagnoli, 2004). This approach is relatively simple and equally applicable, even to complex processes; its primary limitation is that process design is finalized before the controllability analysis is carried out. So, there is a possibility that one might miss out the process design alternative that is better controllable with little additional economic penalty. In addition, the process design, which is finalized based only on steady-state economic considerations, may have severe operational problems. Hence, in the proposed approach, we select a few potential design alternatives (instead of only one) that are worthy of consideration for further controllability analysis. By doing so, the primary limitation of the traditional sequential approach could be avoided. A similar approach has been used by Narraway et al. (1991) to understand the interaction between design and control of a simple process employing mathematical tools on linearized models. However, nonlinear dynamic models are not considered in their study.

The proposed approach is based on heuristics and simulation to achieve synergistic benefits. As heuristics cannot always be relied upon, powerful process simulators are employed as an integral part of this approach, to ensure reliability. Process simulators for dynamic studies were not used extensively in the past. However, recent advancements in the computing technology boosted their capabilities, which, in turn furthered studies on plant-wide analysis (Luyben, 2002). Process simulators offer a good platform to study complex processes more effectively. Hence, the present study is based on a process simulator, namely, HYSYS, which has both the design and control capabilities. The designer can seamlessly move to dynamic mode from steady state, and make use of essentially the same model in both the modes. Such a feature can greatly facilitate studies on integrated design and control especially in the plant-wide context, and, hence, HYSYS is chosen for the present study. However, the analysis is generic and applicable to any other commercial process simulator that has got similar capabilities of design and control. The proposed sequential approach has two stages: (i) process design and (ii) control system design, which are discussed below.

Process Design: Douglas (1988) proposed a heuristic procedure for conceptual process design, which, hereafter, shall be referred to as conventional design procedure (Figure 6.1). This procedure has received widespread attention from academia and industry over the years. One of its key features is to consider recycles in the early stages. Keeping in mind the increasing complexity of chemical processes, Hoo and co-workers (Emets, 2003; Vasbinder et al., 2004; Emets et al. 2006) proposed a modified design procedure, which is essentially a variant of conventional design procedure, by considering recycles towards the end of the hierarchical procedure (Figure 6.1). Their contention is that recycles should be considered in a later stage, based on their own economical merit. The modified design procedure seems to be more logical as it might be difficult to consider recycle decisions in an early stage, because of the lack of information and the uncertainties involved, for several reasons. First, although the recycling of unconverted raw materials is often mandatory as raw materials are usually expensive, it may be wiser not to have recycles in the case of cheaper raw materials (such as water). Second, when the reaction chemistry is complex with multiple reactions and reversible kinetics, it is not easy to decide, in such an early stage, whether it is economical to recycle certain components (especially intermediate products). Third, if the unconverted raw materials are in the gaseous phase and the conversions are relatively high, the recycling decision is largely dependent on the economic feasibility of a compressor. Fourth, recycle decisions also dependent on the optimal conversion, which is usually a plant-wide decision, and may not be known at such an early stage.

Because of the aforementioned reasons, the process alternative without recycle may be more economical at times; this potential alternative and any other variants of it might be overlooked if the design engineer decides to recycle early in the design stage. On the other hand, using the modified design procedure (i.e., by considering the recycles towards the end), one can systematically compare the economic potential of the process with and without the recycle before deciding on it. Hence, the modified design procedure, while retaining all the benefits of the conventional design procedure, allows the designer to explore more alternatives. In the present study, the feasibility of the modified design procedure is critically analyzed using the HDA process as a case-study, and several design alternatives are generated. Possible improvements to the modified design procedure are also suggested. Finally, a few economically attractive alternatives for design are forwarded to the second (i.e., control) stage.

Plant-Wide Control: Luyben’s heuristic method has been widely used to design control systems for highly integrated processes (Luyben et al., 1999). In this method, he proposes to fix the liquid recycle flow in order to avoid snowball effect, which is popularly known as Luyben’s rule. However, there seems to be no agreement among researchers on this rule. For example, Skogestad and co-workers noted that Luyben’s rule seems to have a limited basis (Larsson et al., 2003). Yu (1999) observed that the Luyben’s rule can only transfer the snowball effect from one part of the plant to another part, but it cannot totally eliminate the snowball effect from the plant. He suggested using a balanced control system instead; however, no procedure to arrive at such a system is given. To circumvent these problems, Konda et al. (2005) proposed an integrated framework, based on improved heuristic methodology and rigorous nonlinear simulation tools. In this framework, similar to the analysis in the design stage, recycles are analyzed towards the end of the methodology and necessary action is taken (based on their severity), with the help of simulation tools. This gives flexibility to the designer to examine any possible improvements to compensate for the deterioration of control system performance due to recycles that otherwise would have been overlooked. In the proposed sequential approach, the integrated framework is utilized in the second stage to quickly design efficient control systems for the attractive alternatives obtained in the first stage. A new metric is proposed and used in this study to analyze the dynamic performance of the alternatives. Finally, a suitable design is selected based on both steady-state and dynamic aspects.

The remaining chapter is organized as follows. The next section critically evaluates two hierarchical process design procedures to generate an optimal process design and presents many process design alternatives. Section 6.3 develops control systems for the economically attractive alternatives obtained in the first stage. In section 6.4, critical evaluation and comparison of the performance of control systems of different process alternatives is carried out using the proposed measure, and the impact of process design on PWC decisions is demonstrated. Finally, chapter summary is given in the section 6.5.

6.2 Optimal Process Design

6.2.1. Hierarchical Procedures

Douglas (1988) proposed a hierarchical procedure for conceptual design of chemical processes (Figure 6.1). He then applied this procedure to the HDA process and obtained a design which shall be referred to as conventional base-case design. According to the conventional design procedure, both the reaction system and the recycles are considered in the third stage of the five-stage hierarchical design procedure. As discussed previously, Hoo and co-workers (Emets, 2003; Vasbinder et al., 2004; Emets et al. 2006) proposed a modified design procedure to handle the increased complexity of the chemical processes efficiently (Figure 6.1). The modified design procedure involves two modifications of the conventional design procedure:

(1) The reaction section, being the heart of any chemical process, should be given special attention and included a separate stage for reactor design; and

(2) Recycles should be considered towards the end, but not in early stages, of the design procedure, based on their own economic merit.

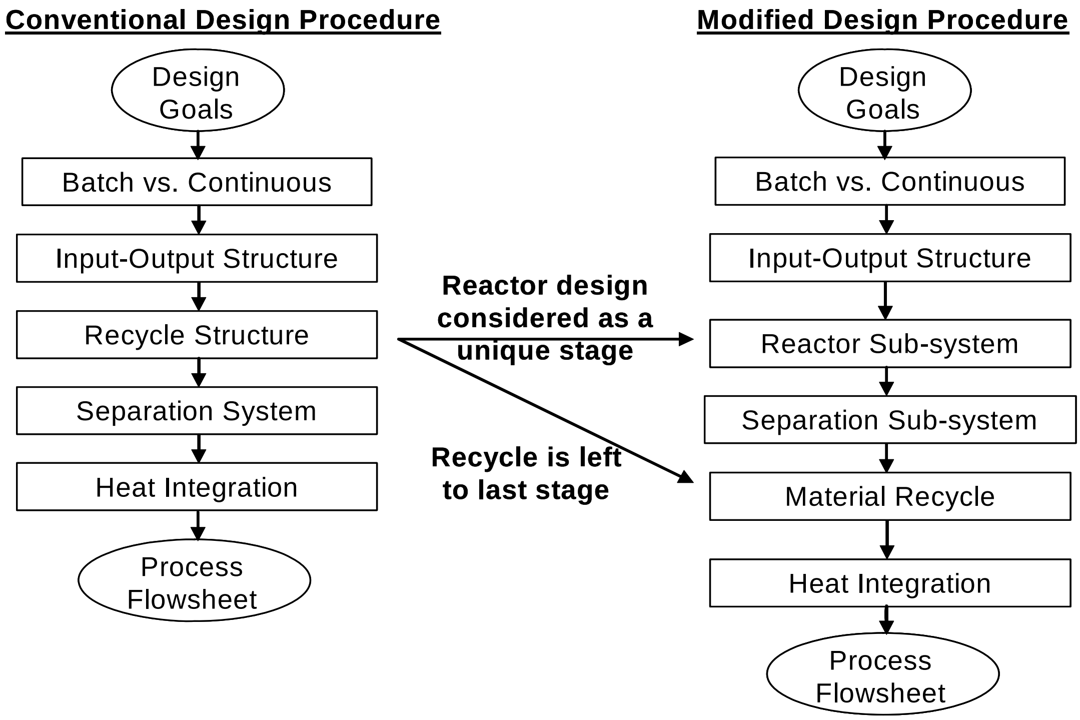


Figure 6.1: Conventional and Modified Design Procedures

By applying the modified design procedure to the HDA process, Emets (2003) was able to obtain a modified process design with two main differences when compared to the conventional base-case design: (i) with a greater emphasis on reaction section, he obtained a reactor scheme that consisted of three reactors in series (Figure 6.2), in contrast to the single reactor obtained by the conventional design procedure, and (ii) with greater emphasis on recycles, he concluded that gas recycle is not needed, for economical reasons. Emets (2003) claimed that the modified design requires less hydrogen and, hence, the modified design procedure is capable of generating a more economical design. However, he considered the “hydrogen-to-toluene ratio in the reactor feed” as the process constraint, whereas the actual process constraint is ‘hydrogen to aromatics (sum of toluene, benzene and diphenyl) ratio in the reactor feed’ (McKetta, 1977; Douglas, 1988). As can be seen from Figure 6.2, with the hydrogen-to-toluene ratio constraint, benzene and diphenyl in the feed to the second and third reactors would not have to be taken into account. Consequently, the hydrogen flow rate in his design is greatly reduced, which led Emets (2003) to conclude that the HDA process with three-reactor scheme is less expensive than the conventional base-case design. Hence, difference in the process constraint is the primary reason for the more economical nature of his modified design.

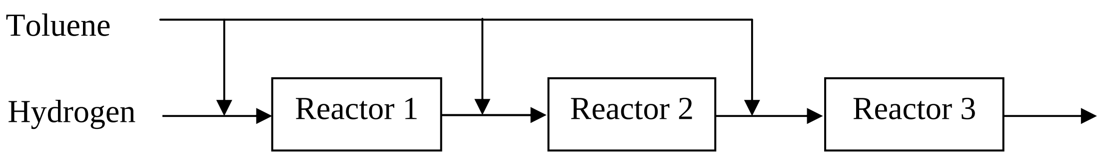


Figure 6.2: Emets’ Modified Reactor Scheme

Based on the aforementioned analysis, one cannot conclude that the modified design procedure is inferior to the conventional design procedure. Had the real constraint been the same as the one assumed by Emets (2003), the conventional design procedure could not have generated the process alternative without gas recycle (which is indeed more economical, as discussed earlier). In other words, the most economical alternative would have been skipped out of designer’s consideration if conventional design procedure were used. Although Emets’ first suggestion, which can be easily incorporated into conventional design procedure (with slightly more emphasis on reaction section during the third stage), the second suggestion regarding recycle analysis deserves further examination before implementing/discarding it. Analyzing the recycle effects towards the end is logical as it would allow the designer to explore more potential alternatives that otherwise would have slipped out of designer’s consideration. For example, if there were no gas recycle in the HDA process, one could think of replacing the stabilizer with a simple flash as methane accumulation within the process is much less now. However, this potential alternative would not have surfaced if one had fixed the recycles early in the design, which puts additional constraints on the possibilities for reactor and separation subsystems. Hence, one of the objectives of this section is to critically evaluate the feasibility and usefulness of the modified design procedure, in comparison to the conventional one.

To apply either of the two procedures listed in Figure 6.1, it is necessary to evaluate the profitability of the different flowsheets generated at each stage of the procedure, so that the designer can select the most profitable alternative(s) and proceed to the next stage. A summary of the profitability analysis is shown in Figure 6.3 and further details can be obtained from Seider et al. (2004) and Turton et al. (2003). Cost correlations are taken from the latter, and a return on investment of 20% is considered to be the profitability measure to calculate the selling price of benzene.

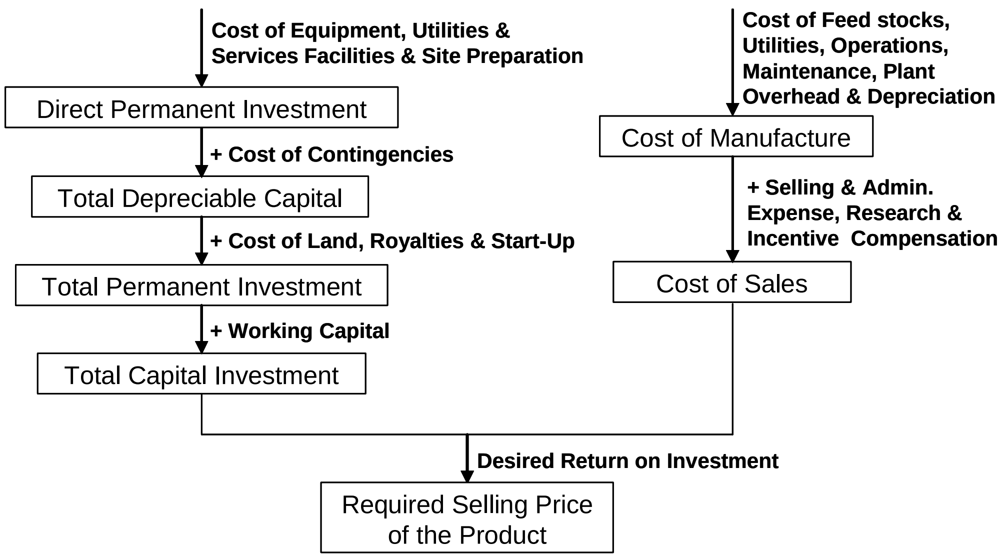


Figure 6.3: Profitability Analysis of a Flowsheet

To facilitate the plant-wide profitability analysis, a custom-made HYSYS-Visual Basic-Excel interface (Figure 6.4) is developed to automate profitability evaluation of a particular flowsheet. It combines the process simulation power of HYSYS with the spreadsheet capabilities of Microsoft Excel program by linking the object libraries of these two applications through Visual Basic. The interface captures the key process simulation results from HYSYS and displays it in a user-friendly interface, allowing the user to see, at one glance, whether all the key process constraints are satisfied. This interface also allows the user to change the simulation parameters in HYSYS directly from Excel. For example, the user can change the desired reaction conversion in the Excel interface, which will automatically transmit the new input to HYSYS, which, in turn, runs the simulation, based on the new input and then send the new results back to the Excel interface. With this interface program, the time taken to evaluate a process flowsheet is greatly reduced, the application of the design procedures becomes simpler, and the results are more accurate.

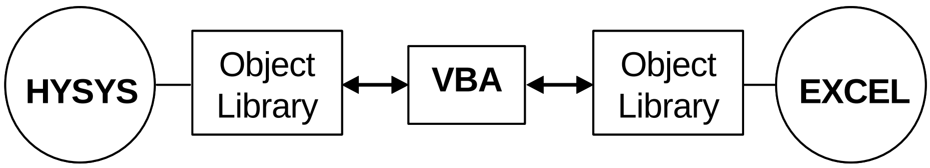


Figure 6.4: Linking Object Libraries of HYSYS and Excel

6.2.2 Application to the HDA Process

Because of space limitations, only those steps that are different from the steps in conventional design procedure are discussed in this section. The main difference between the two procedures arises in stage 3. If one uses the conventional hierarchy, before designing the reactor subsystem in stage 3, decisions would be made on which output streams from the process “black box” in Figure 6.5a are to be recycled. For the case of the HDA process, benzene is obviously removed as a product. Toluene is a valuable reactant, and, hence, it should be recycled to the process. Diphenyl is a byproduct and a decision should also be made in regard to remove it from or to recycle it into the process. If diphenyl is removed from the process, there will be loss of some benzene to diphenyl, and, hence, the toluene consumption and cost would increase. Furthermore, there are the additional capital and operating costs that are associated with the extra separation step of removing the diphenyl. It is also necessary to consider the equilibrium constant of the side-reaction. Finally, a decision is needed as to whether there should be recycle of the gas stream that is rich in hydrogen. Here, a tradeoff exists between the savings in fresh hydrogen and the additional costs associated with the recycle compressor as well as the methane buildup in the loop. It is possible to make rough calculations in order to estimate the economic potential of these alternatives and make decisions in regard to which streams to recycle. By doing so, Douglas (1988) developed the process structure shown in Figure 5a.

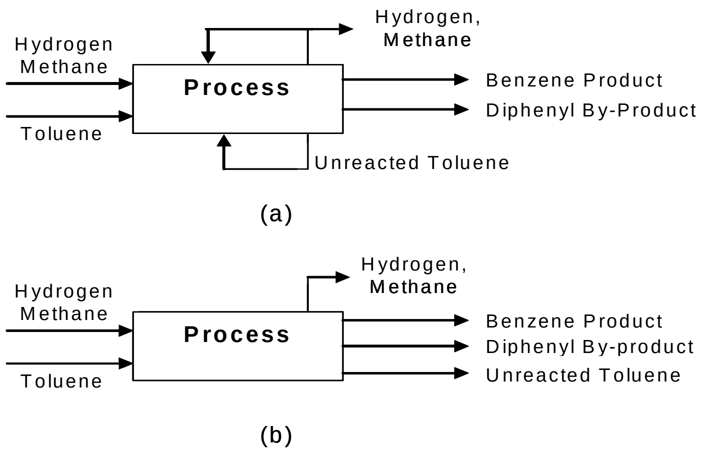


Figure 6.5: HDA Process after Stage 3 of (a) Conventional and (b) Modified Design Procedure

Subsequently, Douglas (1988) continued with the subsequent stages in the conventional design procedure (Figure 6.1) and arrived at the flowsheet given in Figure 6.6. He observed the optimal conversion to be 75%. However, a recent study by Phimister et al. (1999) observed the optimal conversion to be 70%. Hence, we performed plant-wide optimization, using the latest cost data, over a wide range of conversion to find the optimal conversion. The selling price of benzene is observed to be relatively constant ($64.49 - $64.53/kg-mol) in the conversion range of 70% – 75%, whereas the price steeply increases if the conversion is <70% or >75%. This is because, beyond 75% conversion, yield losses are dominant and, recycling costs are observed to be dominant below 70% conversion. In the present study, 70% is used as the optimal conversion for conventional base-case design.

The question with respect to the conventional procedure is how confident one can be about recycle decisions made in stage 3. At such an early stage of the hierarchy, it might not be easy to make decisions in regard to which streams to recycle, based on heuristics or rough calculations. It is more or less certain that toluene, being a valuable feedstock, should be recycled back to the process. However, the decision is not so clear for diphenyl, hydrogen, and methane, because such recycles might have a great impact on the design of the reactor and separation subsystems. For example, if one had decided on recycling the hydrogen/methane stream at stage 3 of the hierarchy, the possibility of replacing the stabilizer column with a simple flash unit due to the elimination of methane buildup in the system might not have surfaced. This shows that potentially more-efficient designs of the reactor and separation subsystems could have been missed if recycle streams were fixed a priori.

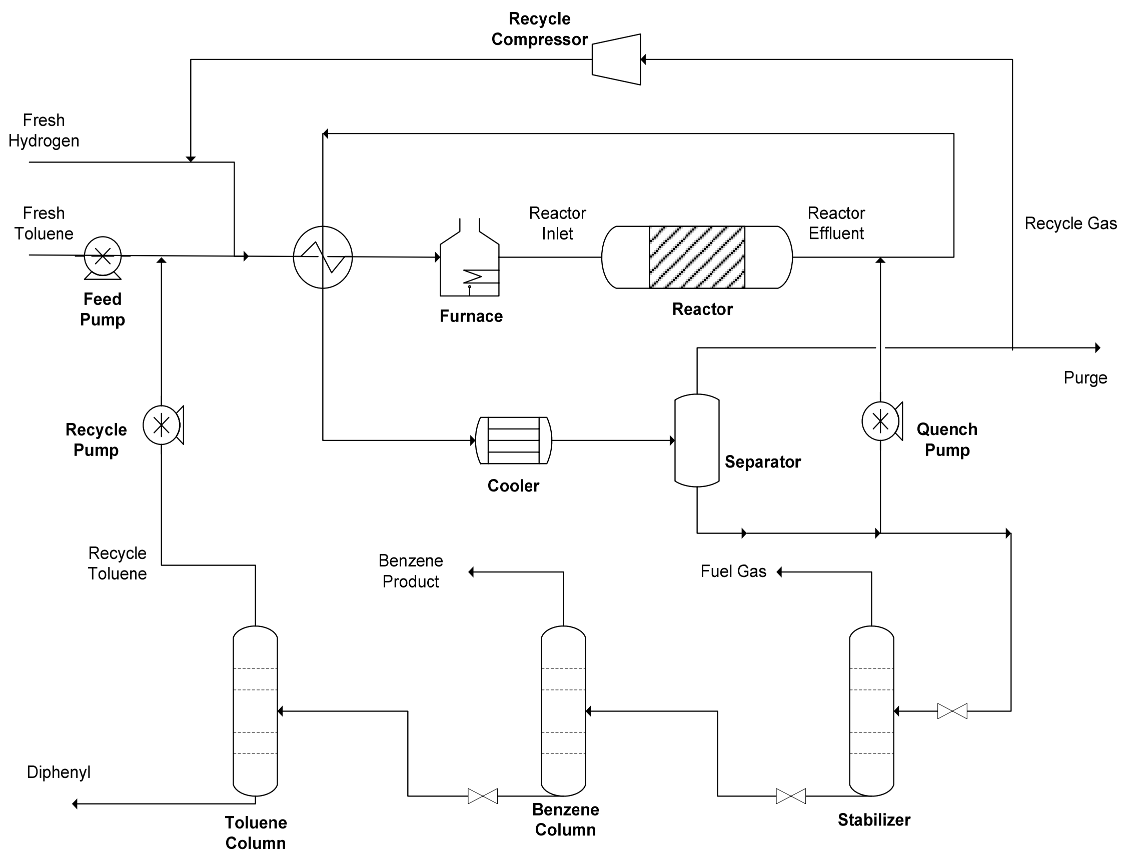


Figure 6.6: HDA Flowsheet from the Conventional Design Procedure

The modified design procedure avoids this limitation of the conventional hierarchy by putting off the recycle decision to a later stage. In this manner, the reactor and separation subsystems can be designed without any limitations and the recycle decision on each output stream can be taken on its own merit, i.e., whether recycling a particular output stream will yield a less-expensive flowsheet than the base flowsheet without any recycle streams. However, we must not neglect the impact of a recycle stream on the reactor and separation subsystems. For example, the decision to recycle diphenyl would mean that the diphenyl concentration in the process would build up to an equilibrium level and, therefore, the concern of increased selectivity losses at high reactant conversions is eliminated. As such, the reactor system can be redesigned to operate at a higher optimal conversion. Therefore, it would be more appropriate to add an iterative loop to the modified design procedure to reflect the re-consideration of the reactor and separation subsystems whenever a new recycle stream is considered (Figure 6.7).

Through application of the modified design procedure (Figure 6.6) to the design of the HDA process, one would logically start by evaluating a flowsheet where diphenyl, excess toluene, hydrogen, and methane are all removed from the process, as shown in Figure 6.5b. However, as previously mentioned, recycle of a valuable feedstock of toluene is almost certainly economical and one might choose a flowsheet with only toluene recycle as the base case instead. This is done in this study and the required benzene price of this flowsheet is found to be $92.7/kg-mol benzene (at an optimum reactant conversion of 95%). This price was then used as the base price for analyzing the next recycle decision.

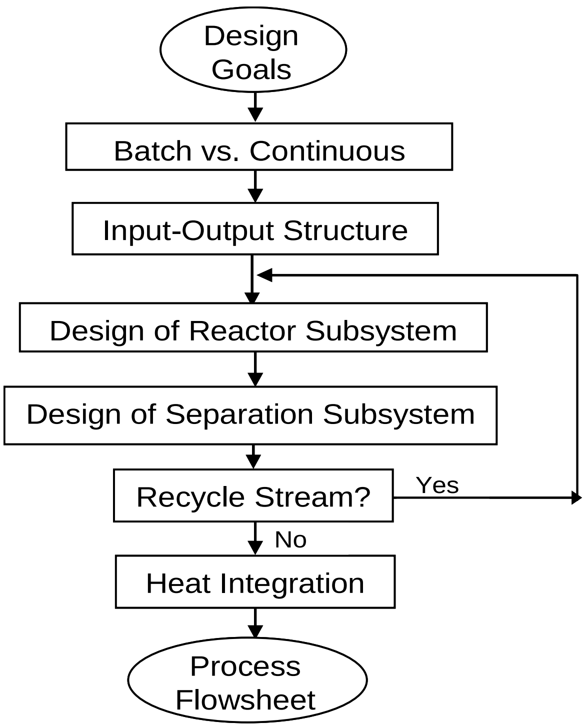


Figure 6.7: Modified Design Procedure with Additional Iterative Loop

As the overall equilibrium constant for diphenyl formation is very low, it might be economical to recycle diphenyl and let it build up in the process to the equilibrium level. In such a case, the capital and operating costs that are associated with the toluene column are removed. Most importantly, selectivity losses are eliminated. Though the fuel value of diphenyl is lost and all the equipment in the liquid-recycle loop has to be oversized to accommodate the increased flow rate, savings in the toluene feedstock are expected to be more significant. Moreover, the optimum reactant conversion is expected to be higher than that of the conventional base-case design, as there is no selectivity loss. Hence, as observed by Douglas (1988), the optimum reactant conversion for this alternative can even go as high as 98%. From the economic analysis of recycling diphenyl to extinction, the selling price of benzene is found to be $88.6/kg-mol (at an optimum reactant conversion of 98%). This price is lower than the base price, and, therefore, it is economical to recycle diphenyl.

The option of recycling hydrogen is then examined. Two possible alternatives are:

1. Recycle the gas stream directly without any gas separation unit but with a purge stream to avoid methane accumulation, and
2. Recycle hydrogen-rich stream after a gas separation unit.

For both these alternatives, conversion can be higher than that of the conventional base-case design, as there are no selectivity losses. From the cost split of various units in the process, two of the most expensive unit operations in the HDA process are the reactor and the compressor. Hence, the designer needs to strike the right balance between reactor and compressor costs. For the first alternative, plant-wide optimization is performed to minimize the selling price of benzene ($/kg-mol). Extensive simulations are carried out over a wide range of conversion (from 50% to 98%, with an interval of 5% conversion), and the optimal conversion is found to be 90% for the modified design. However, for this alternative, Douglas (1988) observed the optimal conversion to be 97.7%, which is different from our finding. This variation can be attributed to the changes in the cost of the reactor and the compressor, with them being the two most expensive equipments in the HDA process. Douglas' cost data were updated to the present-day values, for a fair comparison. About 27% hike in reactor cost and about 23% reduction in the compressor cost are observed, which obviously mean that a reactor with less volume and, hence, less conversion (and more recycle) will be more economical, which is consistent with our finding. The selling price of benzene for this alternative is observed to be \$62.7/kg-mol at optimal conversion (90%). This alternative is less expensive than the conventional base case design (\$64.5/kg-mol), despite the fact that it requires a larger reactor (in order to achieve high conversion as there are no selectivity losses). The larger reactor lessens the recycle flows and the controllability is expected to be better. However, the number of recycling components here is more and may result in operational problems. Hence, to gauge the operational benefits of this process design, rigorous nonlinear dynamic simulations should be performed.

For the second alternative, membrane gas separation is considered, as it can be economically competitive with conventional gas separation methods (such as cryogenic distillation, absorption, and pressure-swing adsorption), especially when the product purity requirements are not very high (Kao, 1987; Meindersma, 1991; Scott, 1995). For processes, that require high-purity (> 99.9%) hydrogen, pressure swing absorption can be cost-effective (Meindersma, 1991). However, for the HDA process, the purity requirements on H_2 are not very high, and, hence, membrane separation can be a cost-effective alternative. In addition, the gas flow rate from flash in the HDA process is low ($<10^8$ ft^3/day), and, hence, membrane separation is the most favorable option (Prasad et al., 1994). Several design issues that arise at this stage are:

(1) Which membrane configuration – a simple, recycle-permeator or two-membrane-type permeators, should be considered?

(2) What should be the operating conditions of the membrane purification unit? do the feed conditions (temperature and pressure) require preprocessing?

(3) What are the maximum attainable purity and recovery of hydrogen in the permeate stream?

(4) Where should the membrane unit be placed - on the purge stream or the flash vapor stream?

As the separation of hydrogen and methane is easy because of the higher selectivity (values as high as 200 are reported by Zolandz and Fleming, 1992), a simple membrane-permeator is considered in this study. As the gas feed to the membrane is already available at high pressure (~ 445 psia), no further compression is needed. As the gas feed to membrane is available at low temperature (100 ^oF), polymeric membranes can be used without any difficulty in the operation. Alternatively, one can consider inorganic membranes or mixed-matrix composite membranes (with enhanced desirable characteristics). More than 95% purity and recovery of H_2 can be expected for H_2/CH_4 separation (Scott, 1995; Nakagawa, 1994).

The placement of the membrane unit introduces two more potential design alternatives: place the membrane unit on the entire flash vapor stream or place it on the purge stream. This placement has different economic and operational implications on different sections of the plant (especially the reactor and compression sections). The alternative with the membrane unit on the flash vapor stream has a distinct feature – the methane content in the reactor is reduced to the smallest possible value, which has both positive and negative effects. Owing to the relatively lesser methane content in the reactor section, the required reactor volume would be less and, hence, reactor is less expensive. On the other hand, there is a greater possibility that the reactor outlet temperature would exceed the maximum allowable value due to the reduced methane content in the reactor coupled with the fact that the optimal conversion is relatively high. Recall that methane in the reactor serves as thermal sink to keep the outlet temperature well below the constrained value, as in other alternatives. Consequently, the reactor section has to be modified accordingly, which will be discussed later. Similarly there are differences in the compression section of both the alternatives. Compression costs in the first alternative, i.e., the process with the membrane unit on the flash vapor stream, would be higher as all the relatively high-purity hydrogen (i.e., membrane permeate) has to be compressed to the reactor conditions from very low pressures. Although the second alternative, i.e., the process with the membrane unit on the purge stream, requires two compressors – one to compress the membrane permeate and the other to compress the gas recycle stream (which is already at relatively high pressures), the overall compression cost is expected to be less, compared to the first alternative as the amount of membrane permeate is relatively less. However, the aforementioned merits of the second alternative are dependent on the purge ratio (i.e., what fraction of flash vapor stream is taken out as purge). Hence, both alternatives are analyzed further.

The alternative with the membrane unit placed on the flash vapor is considered first, and brief description of the membrane unit[†] is given as follows. The feed to the membrane is at 445 psia and 100 ^oF. The CH_4-rich retentate is assumed to be leaving at the same temperature and with a small pressure drop (5 psia), and, it can be used a fuel gas. H_2-rich permeate is assumed to be leaving at a much lower pressure (i.e., 45 psia in order to provide a good driving force for separation) and a temperature (95 ^oF) slightly lower than the feed temperature (100 ^oF). Based on the Hydrogen Production Facilities Plant Performance and Cost Comparisons Final

[†] Due to the unavailability of the membrane unit in HYSYS, an extension from the Aspentech support website is used here to simulate the membrane unit.

Report published in March 2002 by Parsons Infrastructure and Technology Group Inc. (http://www.fischer-tropsch.org/DOE/DOE_reports/40465_fr/40465_fr_toc.htm, accessed in April, 2006), a value of 0.1 std cc/min/cm2/cm Hg was used as the hydrogen flux through the membrane. Zolandz and Fleming (1992) suggested an optimal selectivity of 110 for H_2-CH_4 separation, and, hence, it is used in this study. The required membrane area is estimated to be 186 m^2 to achieve 98% pure hydrogen and 98% recovery of hydrogen in permeate. A spiral-wound module, which is relatively less expensive than a tubular module, is considered; alternatively, hollow-fiber modules can be considered, which are much cheaper but they suffer from fouling. The cost of spiral-wound modules can vary between US\$10/m^2 and US\$100/m^2 (Baker, 2002); therefore, an average value of US\$55/m^2 is assumed. With these specifications, the membrane cost is only 0.23% of the overall capital cost, and, hence, any uncertainty in the membrane information will not affect overall conclusions that will be deduced. Although the membrane operation is observed to be relatively inexpensive, one of the problems with membrane operation is that the permeate pressure (usually close to atmospheric pressure) will be well below the feed pressure. Hence, in the HDA process, the permeate compressor is observed to be expensive (almost one-third of the total capital cost), and the operating cost is also significant.

In the conventional base-case design for the HDA process, the excessive methane content in the reactor serves as a heat-sink to maintain the reactor outlet temperature well below the upper limit (1300 ^{0}F) to avoid cracking, although the reactor is adiabatic. However, in the modified HDA process with the membrane unit on the flash vapor stream, the amount of methane within the reactor is significantly less as most of the methane is removed by the membrane unit. Also, as there are no selectivity losses, the optimal conversion for the process with the membrane unit is expected to be higher than that of the conventional HDA process (70-75%). Hence, more energy will be released in the reactor and the outlet temperature of an adiabatic reactor is unlikely to be within the upper limit. Two possible alternatives are (i) a single nonadiabatic reactor, and (ii) two adiabatic reactors in series with toluene feed-split and an inter-stage heater (Figure 6.8). As mentioned previously, the main problem with the alternatives having a membrane separator is that it requires an expensive compressor, which should be compensated by savings that are introduced by membrane separator (i.e., by reducing reactor cost and saving valuable feedstock). The selling price of benzene is found to be \$60.9/kgmol and \$63.2/kgmol (at an optimum reactant conversion of 98%) for the alternatives with a single nonadiabatic reactor and two adiabatic reactors respectively. For the latter alternative, toluene is equally split between the two reactors, which are designed to give equal conversion; this implies that the reactors are in parallel with respect to toluene flow and in series with respect to hydrogen flow (Figure 6.8).

Next, the alternative of the membrane unit on the purge stream is considered. As discussed previously, this alternative has significant methane in the reactor, which acts as a thermal sink, and, hence, a single adiabatic reactor is sufficient. As expected, the required membrane area is now less as the amount of membrane feed is relatively less. Of all the alternatives, this alternative has more number of recycles and poses more convergence difficulties in steady-state. Hence, recycle blocks are placed judiciously to improve the computational efficiency for optimization studies. In general, the higher the conversion, the more economical is the process, and, hence, the optimum conversion is found to be 98%. Unlike the two alternatives that have the membrane unit on the flash vapor stream, there is one more design variable, namely, purge ratio (i.e., the fraction of flash vapor flow that is purged out and sent to the membrane). Therefore, optimization is carried out with the purge ratio as the decision variable. Initially, profitability of the process increases as the purge ratio increases. However, beyond a purge ratio of 0.25, the loss of hydrogen in the purge becomes significant, and the process becomes less attractive as the purge ratio increases further. At an optimal conversion of 98% and purge ratio of 0.25, the selling price of benzene is found to be \$60.0/kg-mol. This alternative, although required relatively larger reactors than those used in other alternatives with a membrane unit, turned out to be cheaper due to the significant cost reduction in compression section.

Table 6.1: Selling Price of Benzene for Several Alternative Process Structures Generated by the Modified Design Procedure (Figure 6.7)

No	Alternative HDA Process Flowsheet and the Optimal Conversion	Selling Price of Benzene (\$/kg-mol)
1	Without gas recycle and with liquid (only toluene) recycle at 95 % conversion	92.7
2	Without gas recycle and with liquid (both toluene and diphenyl) recycle at 98% conversion	88.6
3	Without gas recycle and with liquid (both toluene and diphenyl) recycle and with stabilizer replaced by a flash unit at 98% conversion	91.4
4	With gas recycle (without membrane separation unit) and with liquid (only toluene) recycle (i.e., conventional base-case design of Douglas, 1988) at 70% conversion	64.5
5	With gas recycle (without membrane separation unit) and with liquid (both toluene and diphenyl) recycle at 90% conversion	62.7
6	With gas recycle (with membrane separation unit on flash vapor stream and a single non-adiabatic reactor) and with liquid (both toluene and diphenyl) recycle at 98% conversion	60.9
7	With gas recycle (with membrane separation unit on flash vapor stream and two adiabatic reactors in series) and with liquid (both toluene and diphenyl) recycle at 98% conversion (Figure 6.8)	63.2
8	With gas recycle (with membrane separation unit on purge stream and a single non-adiabatic reactor) and with liquid (both toluene and diphenyl) recycle at 98% conversion	60.0

Overall, the alternatives with membrane gas separation unit are more economical (Table 6.1); of them, alternative 8 is the most economical. This result is consistent with that of Kocis and Grossmann (Kocis and Grossmann, 1989) and Goel et al., (2002) who have optimized the HDA process flowsheet using MINLP. However, in their studies, process design selection was purely based on steady-state analysis; dynamic implications were not considered. Alternative 6 is the next-best alternative followed by alternatives 5, 7, and 4. Although Douglas (1988) studied several of these alternatives, alternatives involving membranes (especially alternatives 6 and 7) have not been studied, perhaps because of the unavailability of design and cost data for membranes at that time. Alternative 3, though not economical, was neither explored nor possible to be explored by the conventional design procedure. The alternatives without gas and/or liquid recycle are more expensive, because the feed stocks cost contribution towards overall cost is high (Figure 6.8).

To conclude, the modified design procedure, while retaining all the benefits of the conventional design procedure, allows the designer to explore more alternatives in a systematic way. One major modification in the modified design procedure is to consider recycles towards the end of the design procedure, based on their own economical merit. This suggestion is not only beneficial from the point of steady-state design but it is also useful for efficient control system design, as discussed in the next section. As PWC analysis is computationally very intensive and requires careful scrutiny of many transients, only the most promising alternatives are considered in the subsequent section. This is justifiable as one would not want to consider very uneconomical processes, irrespective of how well they can be controlled. At this stage, the designer has to choose the alternatives that are worth considering for dynamic analysis. In case of HDA process, alternatives 4 to 8 are more economical, and, so they are forwarded to the next (i.e., control) stage.

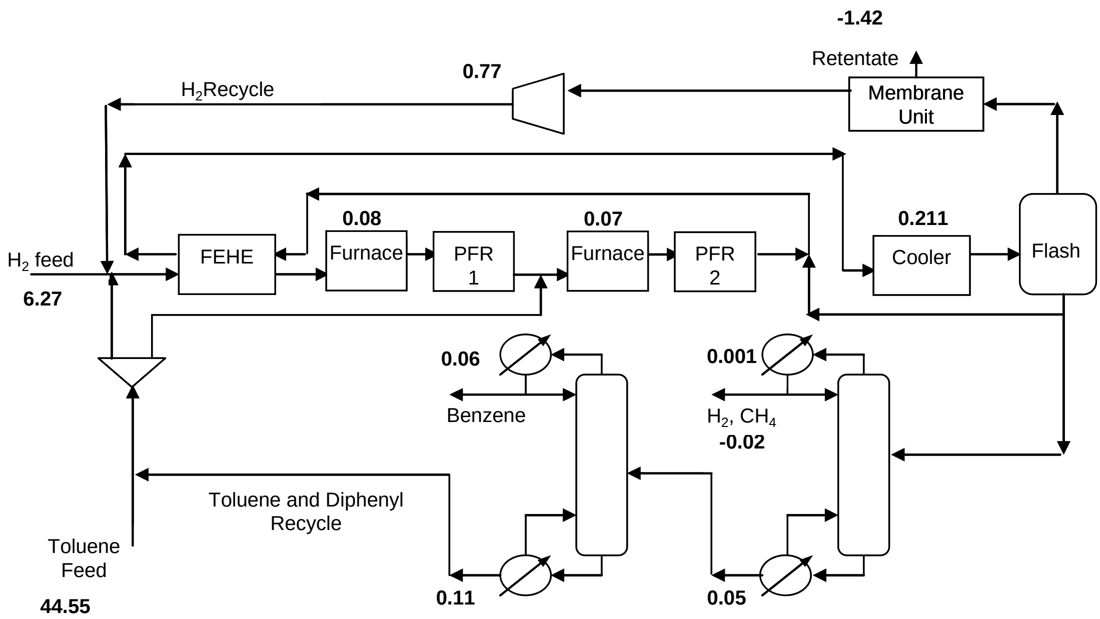


Figure 6.8: Main Operating Costs ($/kg-mol of benzene produced) of Modified HDA Process Design with Membrane Gas Separator (Alternative 7)

6.3 PWC System Design for Promising Process Alternatives

Though recycles are favorable from economic viewpoint, they are notorious from the standpoint of PWC; they can complicate process dynamics, thereby affecting the performance of the overall control system (Kumar and Daoutidis, 2002). Hence, control engineers should explicitly consider the effect of recycles when designing control systems. Konda et al. (2005) proposed an integrated framework in which the severity of recycles is systematically analyzed towards the end of the control system design procedure, very similar to the analysis in the design stage previously presented. The basic idea is to carry out simulations for the process with recycle and without recycle (Figure 6.9) and compare their dynamics in order to understand and rectify the problems caused by each recycle. Because of space limitations, the integrated framework (Table 6.2) is not discussed here. In stage 1 of this framework, CDOF have to be identified. Traditionally, the number of equations and the number of variables are counted to compute CDOF. However, such a procedure is tedious for complex processes with hundreds to thousands of equations and variables. Hence, the method reported by Konda et al. (2006) is used here to determine the CDOF of the alternatives for which the control system has to be developed.

Analysis pertaining to recycles (stage 7 of integrated framework) is briefly described. For this analysis, one should first develop the control system for the process without recycles (Figure 6.9b), which is relatively easier. Its performance should then be analyzed for anticipated disturbances. Similar analysis should then be performed for the process with recycles (i.e., by closing one recycle loop at a time) as in Figure 6.9a. The control system designed thus far may not be satisfactory after closing the recycle loop. Two possible cases are as follows.

CASE 1. Unstable closed-recycle-loop system: The closed-recycle-loop system (i.e., after closing the recycle loop) can be unstable, which is possible as recycles are notorious due to their positive feedback effect. In this case, recycle dynamics are severe enough to make the closed-loop system unstable.

CASE 2. Deterioration in the performance of the closed-recycle-loop system: The closed–recycle-loop system might be stable but there can be loss of performance. By comparing the performances of the systems with and without recycle loop(s), two possible scenarios can be identified: (a) recycle dynamics are severe enough if the performance of the closed-loop system is observed to be much lower, and (b) recycle dynamics are not severe if the closed-recycle-loop performance is comparable to that of the open-recycle-loop.

In Case 1 and Case 2(a), the control system needs to be troubleshot. One should re-configure the control structure. For example, one can make use of the process variables that are largely affected by recycles in the control structure. By doing so, one will have better control over recycle dynamics, thereby improving the overall control system performance.

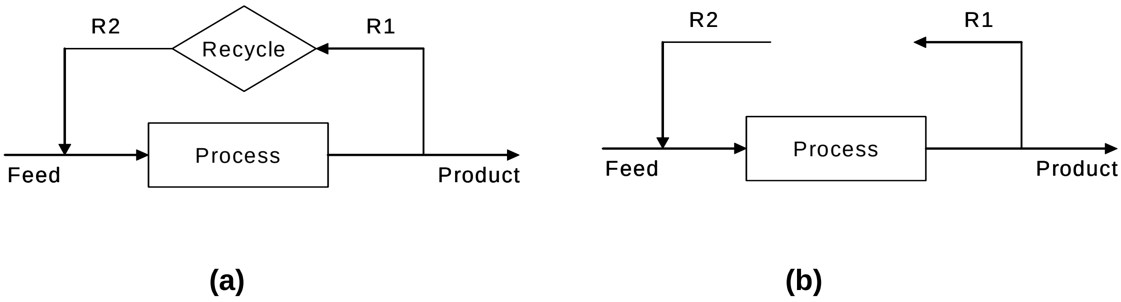


Figure 6.9: Schematic showing (a) Process with Recycle (closed-recycle-loop process) and (b) Process without Recycle (obtained by removing the recycle block). In case (b), streams R1 and R2 will still have base case steady-state values. Removal of stream R2 is not desirable as the process will then have entirely different behavior.

The integrated framework (Table 6.2) is used here to develop PWC systems for the chosen alternatives after the process design stage. Though several researchers used HDA process as the case study to design PWC system, their studies are mainly on the conventional base-case (alternative 4). However, it is evident from the analysis in the previous section and Table 6.1 that process alternatives that are more economical than alternative 4 do exist. However, steady-state optimality does not necessarily guarantee dynamic operability (Chodavarapu and Zheng, 2002). In other words, steady-state feasibility is only a necessary condition, but not sufficient condition, for dynamic controllability. Hence, in this section, PWC systems are designed for alternatives 4 to 8, to investigate their operability and the effect of process design on PWC decisions. One main operational objective in HDA process is to maintain product purity at 99.99 ± 0.01 mol% of benzene. Additional objectives are discussed in the work of Konda et al. (2005).

Table 6.2: Improved Heuristic Methodology (Konda et al., 2005)

Level	Things that need to be dealt with
1	1.1. Define Plant-Wide Control Objectives
	1.2. Determine Control Degrees of Freedom
2	2.1. Identify and Analyze Plant-Wide Disturbances
	2.2. Set Performance and Tuning Criteria
3	**Product Specifications**
	3.1. Production Rate Manipulator Selection ➢ Identify Primary Process Path ✓ Implicit/Internal Manipulators ✓ Explicit/External Manipulators • Fixed Feed Flow Control • On-Demand Control
	3.2. Product Quality Manipulator Selection
4	**“Must-be controlled” Variables**
	4.1. Selection of Manipulators for More Severe Controlled Variables ➢ Process constraints (equipment and operating constraints, safety concerns, environmental regulations) especially those associated with reactor
	4.2. Selection of Manipulators for Less Severe Controlled Variables ➢ Material Inventory – Levels for Liquid & Pressures for Gases ✓ Levels in Primary Process Path – Make sure the control will be self-consistent ✓ Levels in Side Chains – Make sure that the control structure will direct the disturbances away from the primary process path ✓ Pressures in the process
5	**Control of Unit Operations**
6	**Check Component Material Balances**
7	**Effects Due to Integration (i.e., Due to Recycles)**
	Identify Presence of Snow Ball Effect and Analyze it’s Severity ➢ Analyze the need to fix composition in the recycle loop to arrive at a balanced control structure ➢ Or, is it necessary to fix a flow at a strategic position in the recycle loop?
8	**Enhance Control System Performance, if possible.**

6.3.1 Dynamic Performance Analysis

Before describing control system design for alternatives 4 to 8, measures of its performance analysis are first discussed as these are needed for choosing control design options. Luyben and co-workers (Elliott and Luyben, 1995, 1996 & 1997) proposed capacity-based approach to measure the dynamic performance of alternative designs by computing the loss in capacity due to off-spec production; the measure is thus related to product quality regulation. Though capacity-based approach is a useful and practical measure, it cannot be applied in all situations. For example, according to this approach, the off-spec product is assumed to be disposed. However, it may be economical to recycle it as the raw materials are usually expensive. Otherwise, yield-losses will be there and additional costs due to disposal of the off-spec product may render the process economically unattractive. Though it is possible to implement this feature in the capacity-based approach, it cannot be generalized. It may not be desirable to recycle the overpurified off-spec product (although the underpurified off-spec product need to be recycled) as it unnecessarily incurs additional costs. Even if the off-spec product has to be recycled, the recycling location and reprocessing cost will be process-specific. If the off-spec product is due to light impurities, it has to be recycled back to the light-component (impurity) purification section; otherwise, it has to be processed through the heavy-component (impurity) purification section. At times, the off-spec product can not be recycled due to capacity limitations (Zheng and Mahajanam, 1999; Mahajanam and Zheng, 2002), but it has to be stored (for future processing), which incurs additional inventory costs. Thus, the reprocessing cost of the off-spec product will be different in each of these cases, and no generally accepted procedures are available to estimate it. One can assume some cost, but the results will be dependent on this assumed value.

Product quality is important but it can not be the only measure. For example, using capacity-based approach and product quality as the measure, two alternative designs will be dynamically equally good if both are capable of producing on-spec product. However, this need not necessarily always be true. Consider product quality regulation in the case of alternatives 5 and 7 to be discussed in the next section; there is essentially no difference in the product quality regulation in the presence of feed quality disturbance (Figure 6.10). However, the same disturbance has a significantly different impact on the dynamics of other process variables in the two alternatives (Figure 6.11) that are not captured in the product quality profile (Figure 6.10). Hence, product quality regulation is only necessary but not sufficient to be considered as an overall performance measure. In addition, the ultimate decision on relative performance is likely to be biased on the performance of the product quality loop (i.e., its manipulator and tuning) if one uses capacity-based approach as the overall performance measure. On the similar front, production rate also cannot be an appropriate measure for the overall performance. For example, on-demand control has better product-regulation capability, but its dynamic performance is not as good as a fixed-feed control strategy (Luyben, 1999). On the other hand, if all control loops are included to measure the plant-wide performance, the analysis can be tedious. Though it is possible to introduce weighting factors for the performance of each loop to compute an overall performance metric, the weighting factors are subjective.

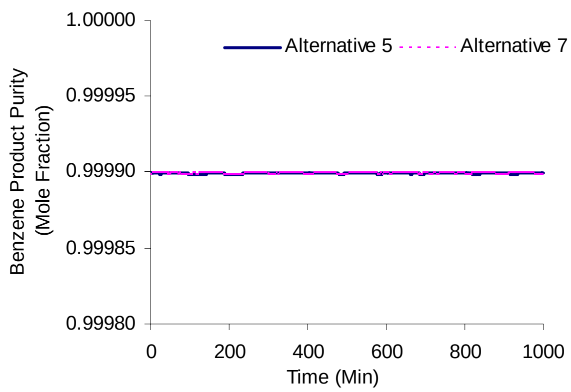


Figure 6.10: Transient Responses of Benzene Product Purity in Alternatives 5 and 7, for -2.5% Variation in Hydrogen Feed Concentration

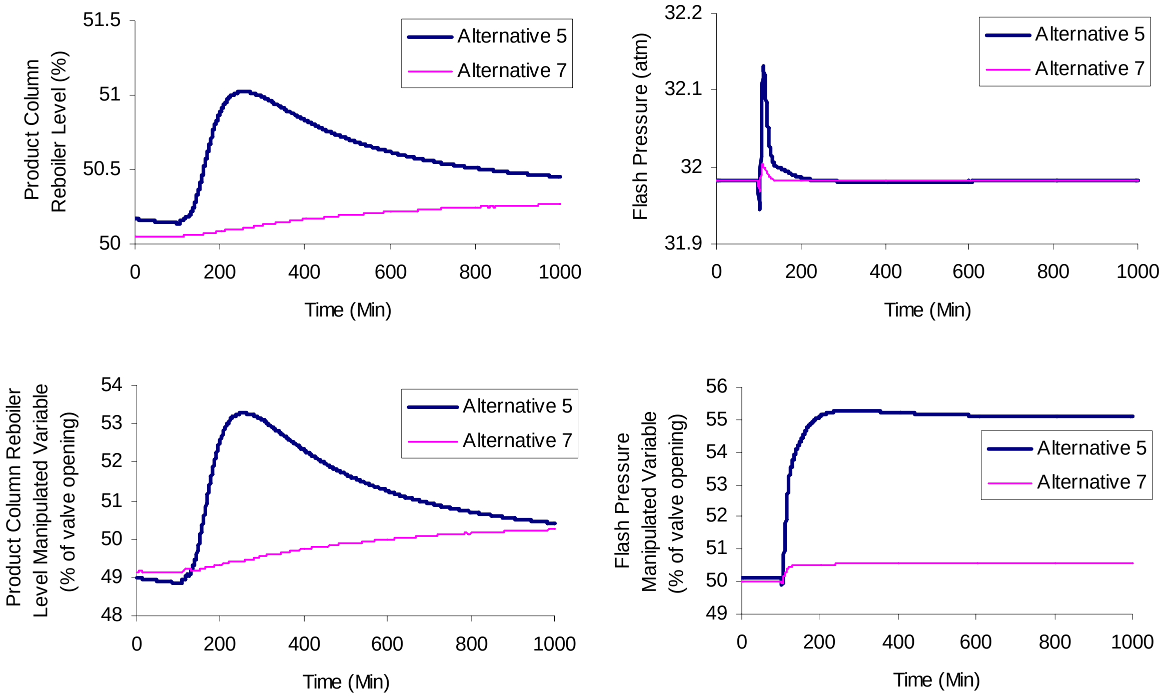


Figure 6.11: Transient Responses of Some Process Variables and the Corresponding Manipulated Variables of Alternatives 5 and 7

To circumvent the aforementioned difficulties, a new performance index is proposed in the present study. Through extensive simulations, we have identified that the overall control system performance and component accumulation (or depletion; i.e., rate of change) are strongly correlated. In the presence of disturbances, accumulation is not equal to zero for a certain period of time until the effect of disturbance is attenuated by the control system. Obviously, the process does not reach steady-state until and unless the accumulation is zero. Indeed, all controlled variables (and, thus, the manipulated variables) in the process are found to reach steady-state if and only if the accumulation of all components reaches zero. Thus, the integral of absolute accumulation can serve as the impact of disturbance on the process. Absolute accumulation is considered since neither positive nor negative (i.e., depletion) value is desirable. Consequently, accumulation profiles of all components are plotted and the absolute area under the curve is used as a measure of PWC performance. Naturally, the lesser the area, the better is the control and the corresponding alternative. As this measure essentially quantifies the effect of disturbance on the process dynamics, integral of absolute accumulation of all components will be referred as the "Dynamic Disturbance Sensitivity (DDS)". For example, for a -2.5% variation in the hydrogen feed concentration, the impact of the disturbance on all the process variables (some of which are shown in Figure 6.11), which was not captured by the product quality profile (Figure 6.10), is captured by the DDS profile (Figure 6.12). Hence, the DDS, based on accumulation, is a better measure of plant-wide dynamic performance.

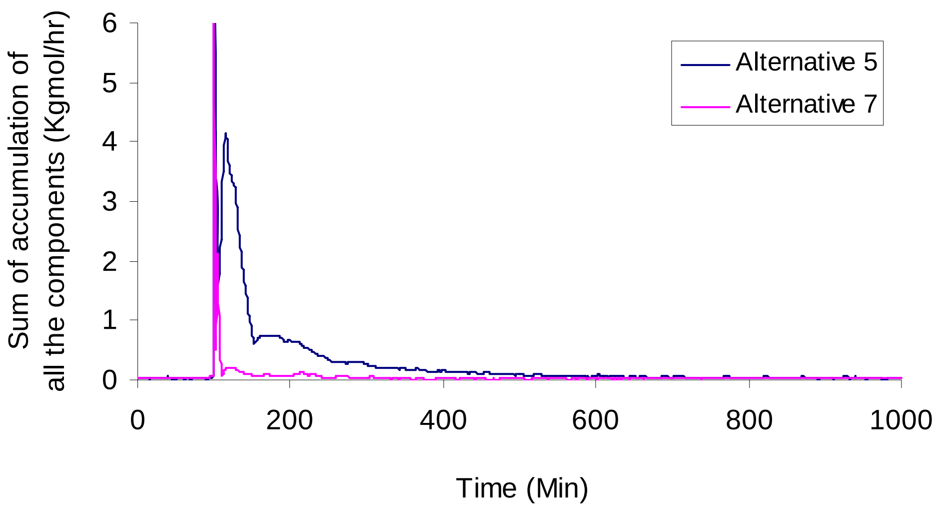


Figure 6.12: Sum of Accumulation of All Components for Alternatives 5 and 7, for -2.5% Change in Hydrogen Feed Concentration

In addition to process design screening, DDS can be used to compare the alternative control structures and tuning decisions. Furthermore, the relative impact of the disturbance on different sections of the plant can be quantified using this measure. In contrast to the steady-state disturbance sensitivity analysis, DDS can be useful to measure the stability of the system as well; for an unstable system, DDS will be very large. It can be combined with rigorous nonlinear simulation models. This not only improves the accuracy but also saves time as the designer does not have to linearize the nonlinear models for linear model-based controllability indexes to analyze the performance. DDS is equally applicable to performance analysis for set-point changes. Furthermore, DDS is very useful to assess the dynamics of the process (such as overall time constant) without having to examine all the process variables to identify the slowest-responding one, which, in turn, is dependent on several other factors (e.g., the type of disturbance). In the case of complex processes where large number of alternatives is possible, DDS can quickly screen the alternative control structures and process designs, based on their dynamic performance. In the following sections, it is used to assess the dynamic performance of process design and control alternatives in the presence of several anticipated disturbances. Controller design and tuning is done in the same way as was done in Chapter 5. See section 5.4.2 and Appendix C for more details on controller design and tuning.

6.3.2 PWC System Design for Alternative 4

The PWC system for the conventional HDA process has recently been designed by Konda et al. (2005) and is presented in Chapter 3; therefore, it is not discussed here extensively. They carried out the analysis without the recycles until step 6 and control decisions are taken accordingly. The resulting control structure after step 6 is summarized in Table C.1 (Appendix C). Thus far, the analysis is performed without gas and liquid recycles (i.e., by tearing both the gas and liquid recycle streams). All the control decisions taken so far lead to a control system that is stable even with both of the recycles. However, as shown in the following analysis, a better control system is generated by systematically analyzing the effect of recycles on the overall plant dynamics.

Effect of Gas Recycle on Overall Plant Dynamics: The closed-loop dynamic simulation is run with each of the expected disturbances for the HDA process with and without gas recycle, and the effect of gas recycle on the overall plant dynamics is observed to be negligible when compared to that of liquid recycle. Hence, further analysis is carried out based solely on the impact of liquid recycle on the overall dynamics. The gas recycle contains a purge stream to avoid accumulation of methane in the process; hence, a composition controller is needed to make the methane inventory in the process self-regulating. The composition of the purge stream is controlled by manipulating recycle gas flow. Simulations showed that this composition does not vary much, even in the presence of disturbances. Therefore, one can replace the purge composition controller with a ratio controller (i.e., to maintain the purge flow as a fraction of gas flow) to avoid the use of expensive composition analyzer. In the present study, a composition controller is assumed in the subsequent analysis for alternative 4.

Effect of Liquid Recycle on Overall Plant Dynamics: The two processes, one with liquid recycle and the other without liquid recycle (Figure 6.9), are initially perturbed with two of the most significant and commonly encountered disturbances (i.e., -5% and -25% variation in the toluene feed flow rate). The responses of process variables such as conversion are rated as acceptable or not acceptable, based on how close/far they are to the optimal steady-state values in the presence of disturbances (Table 6.3). In Tables 6.3 and 6.4, variation in conversion and the overall process settling time (taking into account all process variables) are given for a -5% variation in toluene feed flow rate where as the equipment constraints are given for the worst-case disturbance of -25% variation in the toluene feed flow rate. As can be seen from the summary in Table 6.3, the liquid recycle dynamics are severe enough to deteriorate the control system performance significantly, indicating the need for a better control structure. The responses of process variables are then scrutinized, and the conversion is found to be greatly affected by liquid recycle dynamics. Hence, a conversion controller (using the furnace duty as the manipulated variable) is included in the control structure, and the process with recycle and conversion controller is found to be performing much better without hitting any constraints, even in the presence of the worst-case disturbance (last column in Table 6.3). In addition, for a -5% variation in the toluene feed flow rate, DDS for the alternative 4 without and with a conversion controller are 44.92 and 8.17 respectively; thus, conversion controller lessens the impact of disturbances on the process significantly. Hence, the conversion controller is needed for this alternative not only due to economic reasons but also to improve dynamic performance.

Table 6.3: Severity of Liquid Recycle Dynamics of Alternative 4 and Their Effect on PWC System Performance

	Without liquid recycle	**With liquid recycle and without conversion controller**	**With liquid recycle and conversion controller**
Conversion (Measure of Economic Performance)	72% (acceptable)	80% (not acceptable)	70% (acceptable)
Settling Time (Measure of Dynamic Performance)	200 (acceptable)	1000 (not acceptable)	200 (acceptable)
Equipment Constraints (Measure of Safe Operation)	satisfactory	unsatisfactory	satisfactory

6.3.3 PWC System Design for Alternative 5

Without liquid recycle, the process structure for alternative 5 is similar to that for alternative 4. Hence, all of the control decisions that were taken before introducing the recycles (Table C.1 in Appendix C) are still valid, except the control decisions that are related to the toluene column as there is no toluene column in alternative 5. As the alternative 5 has one column less and is operating at relatively higher conversions, the liquid recycle dynamics of alternative 5 are expected to be less severe than that of alternative 4, and the use of conversion controller is questionable in the former. Hence, analysis similar to that in section 6.3.2 is carried out here for alternative 5, to assess the severity of the liquid recycle dynamics.

Alternative 5 with and without liquid recycle is perturbed with -5% variation in the toluene feed flow rate (see the second and third columns of Table 6.4). Alternative 5 without liquid recycle exhibited a slight variation in conversion (2%) and took 400 min to settle at a new steady state. On the other hand, alternative 5 with liquid recycle exhibited slightly more variation in conversion (4%) and took ~700 min to settle. As the variation in the conversion is small, it is difficult to decide whether a conversion controller is needed or not. However, for the worst-case disturbance (-25% variation in the toluene feed flow rate), one of the level control valves in liquid recycle (the benzene reboiler level control valve) approaches the saturation limits (last row in Table 6.4). For practical reasons, it is recommended to operate control valves with at least 10% opening.

In addition, for -5% variation in the toluene feed flow rate, DDS for alternative 5 with and without conversion controller are 6.45 and 10.10, respectively. Similarly, for -25% variation in the toluene feed flow rate, DDS for alternative 5 with and without conversion controller are 30.13 and 40.13, respectively. Thus, the conversion controller lessens the impact of disturbances on the process and offers the balanced nature to the control system, which, in turn, effectively controls the process, even during the worst case scenarios. In this alternative, it is needed mainly to improve dynamic performance. With the conversion controller, alternative 5 is observed to give satisfactory performance (see the fourth column of Table 6.4) for feed flow rate variations. In addition, several other disturbances are tried and the results are analyzed in section 6.4.

Table 6.4: Severity of Liquid Recycle Dynamics of Alternative 5 and Their Effect on PWC System Performance

	Without liquid recycle	**With liquid recycle and without conversion controller**	**With liquid recycle and conversion controller**
Conversion (Measure of Economic Performance)	92% (acceptable)	94% (acceptable)	90% (acceptable)
Settling Time (Measure of Dynamic Performance)	400 (acceptable)	700 (not acceptable)	150 (acceptable)
Equipment Constraints (Measure of Safe Operation)	satisfactory	unsatisfactory	satisfactory

6.3.4 PWC System Design for Alternative 6

As discussed in the previous section, for the process without gas and liquid recycles, the control decisions taken up to stage 6 of the integrated framework (Table C.1 in Appendix C) remain the same. Step 7 involves the introduction of gas and liquid recycles, one by one, to examine their effects on the overall plant dynamics, which are discussed in this section. Introducing gas recycle involves implementation of the membrane control system, which is discussed below.

6.3.4.1 Membrane Dynamics for H_2-CH_4 Separation

Though the dynamics of membrane units (such as reverse osmosis) have been well-studied, membrane dynamics and control studies for gas separation are very much limited. Moreover, the reported studies are on a simple membrane permeator (e.g., Kao and Yan, 1987). Membrane dynamics and control in the context of PWC have not been studied so far. To design a PWC system for HDA process with a gas membrane separator (alternative 6), dynamics (such as the order, gain, time constant(s) and delay) of a H_2-CH_4 membrane separator are needed. These are not available in the literature; it has been stated that gas permeator membranes are relatively insensitive to changes in feed flow rate, feed composition and membrane surface area (Seader and Henley, 1998). Thus, in this study, first-order dynamics with delay is assumed for the membrane unit as it can adequately represent the behavior of a wide range of processes. Perturbation analysis, using the steady-state membrane model, is performed to obtain gains of hydrogen recovery and permeate purity, with respect to changes in feed flow rate and concentration.

Table 6.5: Results of Perturbation Analysis for Membrane Separation System

	Base case	Membrane Feed Flow Rate changed by		H_2 Concentration in Membrane Feed changed by	
		-10%	+10%	-5%	+5%
H_2 Purity in Permeate	97.92	97.69	98.10	97.62	98.82
H_2 Recovery in Permeate	97.35	98.13	96.45	97.02	97.72

The recovery and purity of H_2 in permeate are relatively insensitive to the expected disturbances in the membrane feed flow rate and concentration (Table 6.5). Hence, the dynamics of concentration can be ignored and, therefore, H_2 concentration in permeate is assumed to be constant at 98%. However, though the H_2 recovery in permeate is practically constant, the permeate flow rate changes with the membrane feed flow rate and, therefore, its dynamics have to be considered. Because the dynamic membrane unit operation is not available in HYSYS, a transfer function is introduced to simulate the dynamics due to changes in membrane feed flow rate. The transfer function is built between the component molar flow rate of hydrogen in flash vapor to the molar flow rate of permeate, and the gain is specified as 1, since any change in input causes an equal change in the output. This specification, together with the permeate purity specification (98% H_2), provides 98% recovery of $H_{2,}$ which is close enough to the desired steady-state value (Table 6.5). Time constant and delay are not yet known; in reality, they depend on several issues: the type of membrane module (spiral-wound or hollow fiber membrane), the type of membrane (dense or porous, glassy or rubbery), the type of membrane material (polymer, inorganic or composite), the membrane configuration (simple or recycle), and the permeabilities of the components involved. Because of the lack of this information in the literature, a conservative estimate of 10 min for time constant is assumed, and delay is taken as 10% of the time constant. To account for any uncertainty in these values, several simulations are run with time constants of 1, 5 and 20 min to see its effect on decisions being taken; however, these differences in the overall process dynamics are observed to be insignificant. As the flash temperature is controlled, the temperature of the feed (and that of permeate) are expected to be relatively constant. Hence, the temperature dynamics are ignored. The membrane downstream pressure varies with the permeate flow; a valve is used to simulate the downstream pressure dynamics with flow variations.

6.3.4.2 Control System Design for Gas Membrane

Usually, the membrane feed temperature and pressure are maintained at constant values. However, as the flash temperature is already controlled, there is no need for any additional control over the membrane feed temperature. Though the flash pressure is also controlled using the valve on the flash vapor stream, there can be some fluctuations in the membrane feed pressure in the range of 20-30 psia. However, within this range of fluctuations, the membrane performance is not affected much and, hence, no control loop is needed for membrane feed pressure regulation.

After introducing membrane dynamics and control system, analysis similar to that carried out in sections 6.3.2 and 6.3.3, is done to characterize the severity of the gas and liquid recycle dynamics. It is found that recycle dynamics are not severe as the process is operating at very high conversion (~98%). Therefore, conversion controller is not required for alternative 6.

6.3.5 PWC System Design for Alternative 7

Process structures of alternatives 6 and 7 are very similar; the only difference is that alternative 6 has one nonadiabatic reactor and alternative 7 has two adiabatic reactors in series (Figure 6.13; detailed separation section of alternative 7 is shown in Figure 6.14). Hence, the reaction section control decisions differ, whereas the rest of the control decisions remain the same. The first reactor, which is adiabatic in nature, requires a controller on the reactor outlet temperature as it is an active constraint. Hence, from the control viewpoint, the first reactor should be modified as there is no manipulator to regulate the outlet temperature. For example, the designer can consider a nonadiabatic reactor that was used for HDA process by some researchers in the past (e.g., Kocis and Grossmann, 1989; Goel et al., 2002); this is a feasible alternative because of the availability of high-temperature heat-transfer agents based on molten fluorides (Williams, 2005) and alloys (http://www.ippe.obninsk.ru/podr/tph/eng/labs/lab54.htm#activity; accessed in May 2006). In case any operational problems associated with high-temperature nonadiabatic reactor are anticipated or a high-temperature coolant is not available, the designer may consider operating the first reactor at slightly lower conversions, which may result in some economic penalty, to keep its outlet temperature well below 1300 ^{0}F. This particular example demonstrates the dynamic implications on process design. On the other hand, the second reactor does not require any outlet temperature controller as the significant amount of methane that is produced in the first reactor acts as a thermal sink to keep the outlet temperature well below 1300 ^{0}F. In addition, alternative 7 requires one feed-split controller and one temperature controller at the inlet of the second reactor (Figure 6.13). As the process is operating at high conversion (98%), recycle dynamics are observed to be not very severe, and hence conversion controller is not required for this alternative too.

6.3.6 PWC System Design for Alternative 8

Alternative 8 differs from alternatives 6 and 7 mainly in two dynamic aspects: (i) alternative 8 has one more gas recycle stream, and, hence, dynamics are expected to be slightly more severe; and (ii) at the designed conversion and purge ratio, the reactor outlet temperature for this alternative is much less than 1300 ^{0}F (even for the worst-case disturbance scenario), and, hence, this alternative does not require any control of the reactor outlet temperature. Hence, unlike alternatives 6 and 7, a single adiabatic reactor is sufficient. Recycle dynamics for this alternative are observed to be not severe as the operating conversion is high and hence conversion controller is not needed.

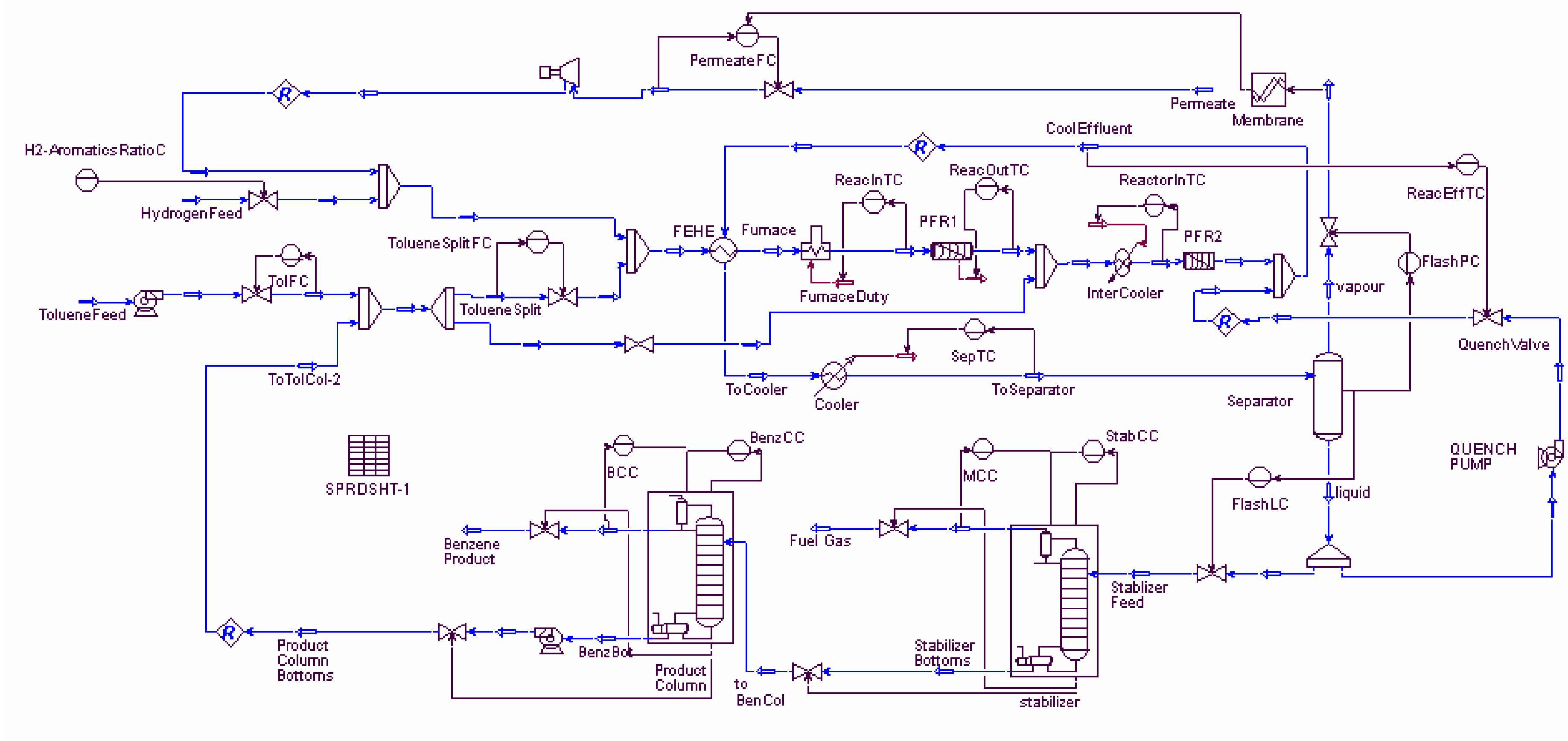


Figure 6.13: Process Flowsheet of Alternative 7 with Control Structure. See Figure 6.14 for detailed control structure for separation section, and Table C.2 (Appendix C) for controllers and their tuning parameters

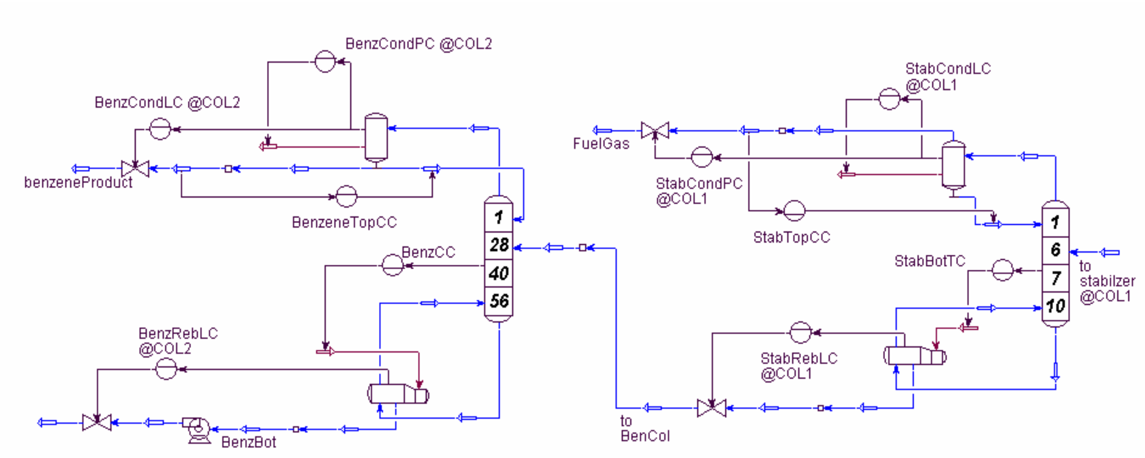


Figure 6.14: Detailed Control Structure of Separation Section of Alternative 7

6.4 Performance Evaluation of PWC Systems of Alternatives 4 to 8

Control systems designed for all five chosen alternatives are evaluated for expected disturbances in feed conditions (i.e., feed flow rate, quality, temperature and pressure) and uncertainty in reaction kinetics. Depending on the type of disturbance, each alternative exhibited significantly different dynamics (Table 6.7). DDS is then used to assess the dynamic performance of these alternatives.

6.4.1 Comparison of Dynamic Performance of Alternatives 4 and 5

Conversion controller for alternative 4 brings significant benefits to the overall control performance (Tables 6.3, 6.4 and 6.6). In general, alternative 5 exhibits faster dynamics than alternative 4. This is mainly due to two reasons: firstly, alternative 5 has one column less in the liquid recycle and hence liquid hold up is less, and, secondly, alternative 5 is operating at higher conversion (90%). In addition, alternative 5 is relatively more robust than alternative 4. For example, in the case of worst-case disturbances, the control valve of a level controller in the liquid recycle loop reaches 5% opening for alternative 5 versus 0% opening for alternative 4. Since it is advisable to operate valves above 10% opening to avoid operational difficulties, conversion controller is still required for alternative 5, which makes the control system even more responsive and robust. However, the benefits of conversion controller for alternative 5 are not as significant as those for alternative 4 (Table 6.6). This is due to the less recycle effects as the process is operating at relatively high conversion. Overall, conversion controller is needed for both the alternatives 4 and 5; alternative 5 is superior to the alternative 4 and observed to be operating closer to the optimal steady-state. As alternative 4 is less economical and has relatively poorer control performance than alternative 5 (see Tables 6.1, 6.3, 6.4 and 6.6), for conciseness, it is excluded from further analysis.

Table 6.6: Comparison of Dynamic Performance of Alternatives 4 and 5

	Alternative 4		**Alternative 5**	
	With Conversion Controller	**Without Conversion Controller**	**With Conversion Controller**	**Without Conversion Controller**
DDS for -5% variation in the Toluene Feed Flow Rate	8.17	44.92	6.45	10.10

6.4.2 Comparison of Dynamic Performances of Alternatives 5 to 8

Alternatives 5 to 8 are subjected to various anticipated disturbances and the control performance results are summarized in Table 6.7. In general, the dynamic performance of each alternative varies with the disturbance. For toluene feed flow rate variation, the performance of all four alternatives is comparable and alternative 7 exhibits slightly superior performance. A similar conclusion can be made for toluene feed temperature variation; in this case, however, the performance of alternative 7 is close to that of the best alternative (alternative 6). In the presence of feed quality variation, alternatives 7 and 5 are observed to be the best and worst performers respectively (Figure 6.15). For hydrogen feed pressure variation, alternative 7 is as good as alternative 6, whereas the poorest performer is alternative 5. In addition, alternative 7 is the only stable process for the disturbances that are related to uncertainty in kinetics. Hence, alternative 7 should be chosen from standpoint of control as it is either superior or competitive with other alternatives for all the anticipated disturbances. Contrary to the general expectation, alternative 7, which is slightly more complex due to the presence of two reactors, is found to be dynamically superior. This may not be recognized without rigorous dynamic simulations. One reason for the superiority of alternative 7 could be the balanced handling of disturbances by the two reactors and, hence, the overall impact of disturbance is less severe.

To conclude, though alternative 8 is found to be the most economical (Table 6.1), dynamic analysis reveals that the alternative 7 exhibits either better or comparable dynamic performance for all of the anticipated disturbances (Table 6.7). In addition, alternative 7 is the only alternative that is stable with regard to uncertainties in the reaction kinetics. As these uncertainties are prevalent, alternative 7 should be the final choice, though it is slightly uneconomical.

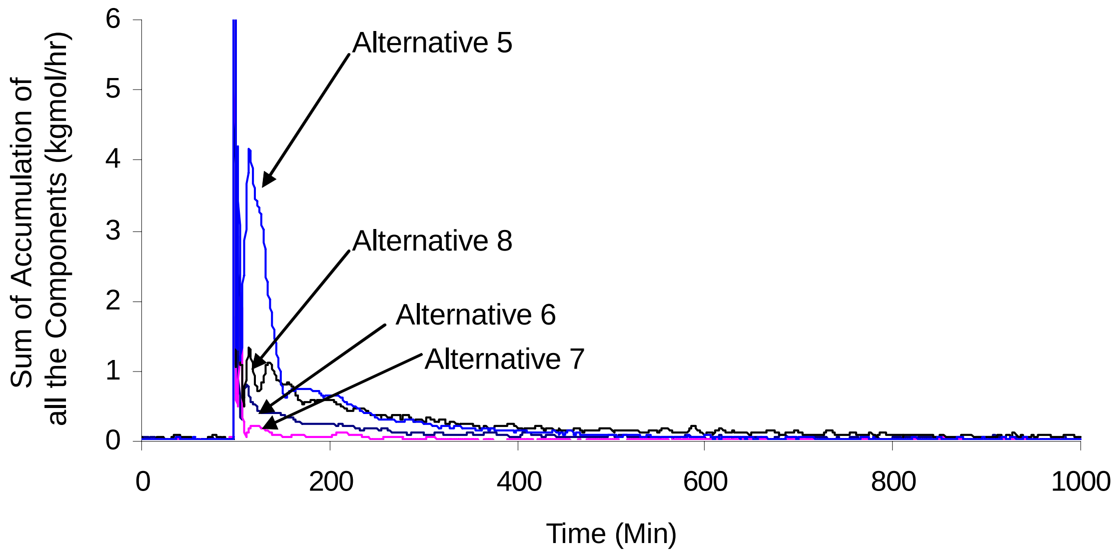


Figure 6.15: Sum of Accumulation of All Components for Different Alternatives

Table 6.7: Performance Assessment of Control Systems for Alternatives 4 to 8

Disturbance		DDS (Integral of Absolute Accumulation of All Components) for				Suggested Alternative(s)
Type	**Magnitude**	**Alternative 5**	**Alternative 6**	**Alternative 7**	**Alternative 8**	
Toluene Feed Flow	-5%	6.45	6.90	5.88	6.11	Alternative 7 is superior
	-25%	30.10	26.23	23.90	24.8	
Hydrogen Feed Quality	-2.5%	4.46	1.88	0.90	3.85	Alternative 7 is superior
	+2.5%	4.28	1.71	1.07	3.07	
Uncertainty in Reaction Kinetics	-5%	Unstable	Valve Saturation	1.87	Valve Saturation	Only alternative 7 should be chosen
	+5%	Unstable	5.47	1.77	3.64	
Toluene Feed Temperature	-10^0C	0.42	0.32	0.39	0.42	Any alternative
	$+10^0C$	0.46	0.31	0.38	0.41	
Hydrogen Feed Pressure	-5%	3.17	0.75	0.81	1.15	Alternatives 6 and 7 are superior
	+5%	1.33	0.51	0.58	0.88	

6.5 Summary

A simulation-based heuristic approach for optimal process design and effective plant-wide control system design is presented and successfully applied to an industrial case study. The modified design procedure, while retaining all the benefits of conventional design procedure, is observed to be effective to surface more design alternatives. For HDA process, the alternatives with the membrane gas separation unit are found to be economically more attractive. However, the dynamic performance of some of them is not as good. In general, dynamic/control performance improves with increasing conversion due to reduced recycle severity. For the process alternatives with relatively lower optimal conversions (alternatives 4 and 5), conversion controller is desirable to improve the dynamic performance. The successful application of the integrated framework of Konda et al. (2005) to several process alternatives demonstrates its capability and generic nature. This study, in general, demonstrates the practicability of the simulation-based heuristic approach for the rigorous treatment of integrated design and control studies for industrial processes. It also emphasizes the conflicts between steady-state economics and dynamic operability, and highlights the importance of integration of design and control from plant-wide perspective. The proposed DDS is observed to be a good measure to quantify the dynamic performance of different process alternatives and control structures. Use of DDS for quantifying the severity of recycle dynamics is under investigation. As discussed in section 6.3.4, due to the unavailability of information on membrane dynamics for gas separations, simplified and yet appropriate dynamics are assumed for the dynamic simulation of process alternatives with membrane units. More accurate simulations require further research on the dynamics of gas membrane units.

CHAPTER 7

CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

PWC system design and several related aspects (such as CDOF, performance assessment of PWC systems, and interaction between design and control) are studied in this thesis. The major contributions and conclusions are as follows.

1. Various PWC methods have been systematically classified based on the ‘approach’ used and the ‘control structure’ considered in each method. This, in turn, would be useful for researchers to quickly understand the two basic features of existing methods and develop newer methods (or tailor the existing methods) to better suit today’s more demanding requirements.
2. A multi-stage integrated framework to design viable PWC systems for industrial processes has been proposed. One of the important features of this framework is to systematically analyze and minimize the impact of recycle, the foe (from control perspective) of many industrial processes, on the overall process dynamics to improve PWC system performance. This framework is then successfully applied to one of the industrially-important petrochemical processes, namely the HDA process. This study demonstrates that the capabilities of process simulators, paired with heuristics can prove to be a boon to PWC of industrial processes.
3. A simple and yet effective procedure for CDOF is proposed and applied to several industrially important processes.

4. A dynamic performance measure, namely DDS, which can be used to assess the performance of alternative control structures and process designs, is proposed. It is then used to show the superiority of the proposed PWC method by comparing the performance of the resulting control system with that of existing control systems in the literature.
5. A modified sequential approach is proposed to study the impact of process design on PWC system by integrating the proposed PWC method and heuristics-based process design procedure. It is shown that the conventional hierarchical process design procedure needs to be modified to better handle the increasing complexity of chemical processes and the corresponding modifications are suggested. The main conclusion here is, though retrospectively obvious but worth repeating as the plant-wide studies in this direction are limited, that the most economically attractive process need not necessarily be the best from operation viewpoint.

7.2 Recommendations for Future Work

PWC is an open-ended problem and there exists scope for many studies. These are outlined below along with some pointers to pursue them.

Application of Proposed Methodology to Other Industrial Processes and Further Enhancements: The proposed methodology has been successfully applied to the HDA process. However, there is a need to apply the proposed method to other processes to enhance it further. Preliminary studies have been carried on styrene and vinyl chloride monomer (VCM) processes, which have shown satisfactory applicability of the proposed integrated framework. Further investigation needs to be carried out to concretize these observations. The most common test-beds for PWC are reactor-separator-recycle (RSR) network and the TE process. For example, more than 60 studies have used the TE process for several applications including PWC, monitoring, fault detection and online optimization (e.g., Ricker, 1995; Duvall and Riggs, 2000; Larsson et al., 2001; Jockenhovel et al., 2003; Tian and Hoo, 2003). On the other hand, till date, there are only a few studies on styrene (e.g., Turkay et al., 1993) and VCM processes (e.g., Seider et al., 2004). It is therefore worth applying the proposed integrated framework to these processes.

In the present study, the main emphasis is given to synthesizing plant-wide decentralized control system with little attention to optimization. So, it is recommended to study the integration of PWC and optimization to further improve profitability by optimally operating the process in the presence of disturbances. This is closely related to plant-wide dynamic optimization or optimal control. A three-tier integration method is proposed by Lu (2003) recently, which can be a good starting point in this direction. Alternatively, it is also possible to integrate self-optimizing control concepts (e.g., Kassidas et al., 2000; Skogestad, 2004) with the proposed framework.

Study of Reactor-Separator-Recycle (RSR) Network: RSR is one of the widely used test-beds to carry out PWC studies as it is simple and yet preserves the general plant-wide nature due to the presence of reactor and separator (either a flash or distillation column) which are interconnected with a recycle. Despite its simplicity, there has not been consensus among researchers on its control strategy - for example, Wu and Yu (1996) suggested a balanced control structure for RSR process by varying reactor holdup (to keep the reactor composition constant) to avoid snowball effect. Loperena et al. (2004), however, identified that the balanced control structure proposed by Wu and Yu (1996) does not eliminate the snowball effect, but transfers it to other process variables. They have then proposed another balanced control structure using the reactor temperature as the manipulator to distribute the impact of disturbance between reactor and separator thereby reducing the snowball effect. Besides, several control structures have been proposed for RSR network. Though all these control structures are valid, one may perform better than the other depending on circumstances. However, clear-cut guidelines are not available on what strategy to be chosen under what conditions. Besides, most of the work on RSR in the past has been based on hypothetical processes with simplified kinetics. In a series of papers, Ward et al. (2004; 2005 & 2006) have recently addressed the impact of kinetics on control policy, which can be a good basis for the work in this direction. In addition, other structural decisions, such as the presence of purge stream, can affect the overall process dynamics (Baldea et al., 2006); the type of reactor holdup (liquid- or gas-phase) also affects the control decisions (e.g., Larsson, 2000). Thus, a more comprehensive study, considering several issues (e.g., presence/absence of purge, type of recycle [gas or liquid], type of reactor holdup [gas, liquid or both], type of reactions [reversible/irreversible/auto-catalytic]), and their effects on overall process dynamics and control decisions, needs to be carried out, using nonlinear dynamic simulations. Steady-state and dynamic models for ethylene- and propylene-glycol processes have already been developed as part of this work (Appendix D), and can be used to carry out further study.

Plant-Wide application of advanced control techniques like MPC: The main emphasis in this thesis is to synthesize a basic regulatory control system based on PID controllers but advanced control techniques (such as MPC or its variants like DMC) are not considered. This is justifiable as the regulatory control system is the basic criterion even for the advanced control techniques. Having successfully developed the basic regulatory control system for the HDA process, the next step would be developing advanced control strategies for the entire plant. In general, plant-wide application of advanced control techniques are relatively limited (Doyle et al., 1997). An attempt in this direction is by Ricker and Lee (1995) who applied nonlinear model predictive control to the TE process. Later, Ricker (1996) observed that the NMPC has only a marginal improvement over the decentralized control system. He has also observed that the decentralized control system does a better job of handling constraints – an area in which NMPC is reputed to excel. So, it is of interest to see whether the advanced control techniques can improve the performance over the regulatory control system in the case of the highly integrated HDA process. Lately, Gonzalez et al. (2006) applied MPC to heat-exchanger networks. One main commonality between any PWC problem and heat-exchanger network control problem is that both of them are highly integrated with the presence of recycles. Thus, the work by Gonzalez et al. (2006) can be a good starting point in this direction.

In general, plant-wide implementation of a single MPC may not always be feasible due to computational limitations, implementation and other practical difficulties (Vadigepalli and Doyle, 2003; Baldea et al., 2006). These difficulties include, but not limited to, insufficient information and difficulty in obtaining the models of certain process phenomena. So, it is often recommended to implement multiple MPCs instead, which is known as decentralized or cooperative plant-wide MPC. In this approach, co-ordination among different MPCs is important to achieve satisfactory overall performance. Recently, Cheng et al. (2005) have proposed a price-driven approach to efficiently co-ordinate decentralized MPCs, and Motee and Rodsari (2003) presented an algorithm for optimal partitioning; these can form a basis for further work in this direction. Another challenging aspect of this study is the identification of plant-wide models to implement MPC.

Economic Quantification of Dynamic Performance: Though interaction between design and control is studied in this work (Chapter 6), economic quantification of the dynamic performance is not explicitly used as there is only one process design alternative which is dynamically stable (for all the anticipated disturbances) for this case study (i.e., the HDA process). However, there may be more than one process alternative which are dynamically stable for other case studies. Hence, to make this study more comprehensive and generic, it is very much needed to economically quantify dynamic performance, which eventually helps to better understand the interaction between design and control. Zheng and Mahajanam (1999) proposed a method to quantify the cost associated with dynamic controllability based on minimum additional surge capacity that is required to meet all of the control objectives and constraints dynamically for all of the expected disturbances, which is a good starting point to work in this direction. The basic idea is to economically quantify the dynamic performance using DDS so that it can appropriately be integrated with the proposed approach to study interaction between design and control.

REFERENCES

Alhammadi, H. Y.; Romagnoli, J. A. Process Design and Operation: Incorporating Environmental, Profitability, Heat Integration and Controllability Considerations. In The Integration of Process Design and Control, ed by Seferlis, P. and Georgiadis, M. C., pp. 264-305. Elsevier: Amsterdam. 2004.

Baker, R. W. Future Directions of Membrane Gas Separation Technology, Ind. Eng. Chem. Res., *41*, pp. 1393-1411. 2002.

Balasubramanian, P.; Kosuri, M. R.; Pushapavanam, S.; Kienle, A. Effect of Delay on the Stability of a Coupled Reactor-Separator System, Ind. Eng. Chem. Res., *42*, pp. 3758-3764. 2003.

Baldea, M.; Daoutidis, P.; Kumar, A. Dynamics and Control of Integrated Networks with Purge Streams, AIChE J., *52*, pp. 1460-1472. 2006.

Banerjee, A.; Arkun, Y. Control Configuration Design Applied to the Tennessee Eastman Plant-Wide Control Problem, Comput. Chem. Eng., *19*, pp. 453-480. 1995.

Barrero, L.; Canales, R.; Romero, D. J.; Mendoza, Y.; Ruiz, G.; Gutierrez, S. S ; Systematic Building-Testing of Dynamic Models for Training Simulators, Comput. Chem. Eng., *27*, pp. 1421-1430. 2003.

Benyahia, F. Flowsheeting Packages: Reliable or Fictitious Process Models?, Trans. IChemE., *78* (Part A), pp. 840-844. 2000.

Bequette, W. B. Process Control: Modeling, Design and Simulation. New Jersey: Prentice Hall. 2003.

Bildea, C. S.; Dimian, A. C.; Iedema, P. D. Nonlinear Behavior of Reactor-Separator-Recycle Systems, Comput. Chem. Eng., *24*, pp. 209-215. 2000.

Bishop, T.; Chapeaux, M.; Jaffer, L.; Nair, K.; Patel, S. Ease Control Valve Selection, Chem. Eng. Prog., November, pp. 52-56. 2002.

Blevins, T. L.; McMillan, G. K.; Wojsznis, W. K.; Brown, M. W. Advanced Control Unleashed: Plant Performance Management for Optimum Benefit. pp. 41-42, NC: ISA. 2003.

Buckley, P. S. Techniques of Process Control. New York: Wiley. 1964.

Cao, Y., Biss, D.; Perkins, J.D. Assessment of Input-Output Controllability in the Presence of Control Constraints, Comput. Chem. Eng., *20*, pp. 337-346. 1996.

Cao, Y.; Rossister, D.; Owens, D. Input Selection for Disturbance Rejection under Manipulated Variable Constraints, Comput. Chem. Eng., *21*, pp. S403-S408. 1997.

Cao, Y.; Rossister, D. An Input Pre-Screening Technique for Control Structure Selection, Comput. Chem. Eng., *21*, pp. 563-569. 1997.

Cao, Y.; Rossister, D. Input Selection and Localized Disturbance Rejection, J. Process Control, *8*, pp. 175-183. 1998.

Carlson, E. C. Don't Gamble with Physical Properties for Simulations. Chem. Eng. Prog. 1996, 37-46.

Castro, J. J.; Doyle III, F. J. Plantwide Control of the Fiber Line in a Pulp Mill, Ind. Eng. Chem. Res., *41*, pp. 1310-1320. 2002.

Castro, J. J.; Doyle III, F. J. A Pulp Mill Benchmark Problem for Control: Application of Plantwide Control Design, J. Process Control, *14*, pp. 329-347. 2004.

Chen, R.; McAvoy, T. Plantwide Control System Design: Methodology and Application to a Vinyl Acetate Process, Ind. Eng. Chem. Res., *42*, pp. 4753-4771. 2003.

Chen, Y. H.; Yu, C. C. Design and Control of Heat-Integrated Reactors, Ind. Eng. Chem. Res., *42*, pp. 2791-2808. 2003.

Chen, R.; McAvoy, T.; Zafiriou, E. Plantwide Control System Design: Extension to Multiple-Forcing and Multiple-Steady-State Operation, Ind. Eng. Chem. Res., *43*, 3685-3694. 2004.

Chen, J.; Adomaitis, R. A. An Object-Oriented Framework for Modular Chemical Process Simulation with Semiconductor Processing Applications, Comput. Chem. Eng., *30*, pp. 1354-1380. 2006.

Cheng, R.; Forbes, F.; Yip, W. S. Price-Driven Coordination for solving Plant-Wide MPC Problems. In Proc. 16th International Federation of Automatic Control, July 2005, Prague, Czech Republic.

Cheng, Y. C.; Yu, C. C. Effects of Process Design on Recycle Dynamics and its Implication to Control Structure Selection, Ind. Eng. Chem. Res., *42*, pp. 4348-4365. 2003.

Chien, I. L.; Zeng, K. L.; Chao, H. Y. Design and Control of a Complete Heterogeneous Azeotropic Distillation Column System, Ind. Eng. Chem. Res., *43*, pp. 2160-2174. 2004.

Chodavarapu, S. K.; Zheng, A., Control System Design for Recycle Systems, J. Process Control, *11*, pp. 459-468. 2001.

Chodavarapu, S. K.; Zheng, A. A Definition of Steady-State Plant-Wide Controllability. Ind. Eng. Chem. Res., *41*, pp. 4338-4345. 2002.

Cole, J. D. and Yount, K. B. Applications of Dynamic Simulation to Industrial Control Problems, ISA Trans., *33*, pp. 11-18. 1994.

Conradie, A. V. E.; Aldrich, C. Neurocontrol of a Ball Mill Grinding Circuit Using Evolutionary Reinforcing Learning, Miner. Eng., *14*, pp. 1277-1294. 2001.

Cuellar, B. D. M.; Villa, M. V.; Puebla, H.; Ramirez, J. A. Model Approximation for Dead-Time Recycling Systems, Ind. Eng. Chem. Res., *44*, pp. 4336-4343. 2005.

Davidson, J.; Bertele, O. V. Process pump selection: a systems approach. Bury St. Edmunds: Professional Engineering Publishing Limited. 2000.

Denn, M. M.; Lavie, R. Dynamics of Plants with Recycle, Chem. Eng. J., *24*, pp. 55-59. 1982.

Dimian, A. C.; Groenendijk, A. J.; Iedema, P.D. Recycle Interaction Effects on the Control of Impurities in a Complex Plant, Ind. Eng. Chem. Res., *40*, pp. 5784-5794. 2001.

Dimian, A. C. Integrated Design and Simulation of Chemical Processes. Boston: Elsevier. 2003.

Diwekar, U. M.; Madhavan, K. P. BATCH-DIST: A Comprehensive Package for Simulation, Design, Optimization and Optimal Control of Multicomponent, Multifraction Batch Distillation Columns, Comput. Chem. Eng., *15*, pp. 833-842. 1991.

Douglas, J. M. Process Operability and Control of Preliminary Designs. In Chemical Process Control – II, Proceedings of Engineering Foundation Conference, ed by Seborg, D. E. and Edgar, T. F., 1981, Sea Island, Ga. pp. 497-524.

Douglas, J. M. A Hierarchical Decision Procedure for Process Synthesis, AIChE J. *31*, pp. 353-362. 1985.

Douglas, J. M. Conceptual Design of Chemical Processes. New York: McGraw-Hill. 1988.

Doyle III, F. J.; Pekny, J. F.; Dave, P.; Bose, S. Specialized Programming Methods in the Model Predictive Control of Large Scale Systems, Comput. Chem. Eng., *21*, pp. S847-S852. 1997.

Downs, J. J. Distillation Control in a Plantwide Control Environment. In Practical Distillation Control, ed by Luyben, W. L., pp. 413-439. New York: Van Nostrand Reinhold. 1992.

Downs, J.; Vogel, E., A Plantwide Industrial Process Control Problem, Comput. Chem. Eng., *17*, pp. 245-255. 1993.

Duvall, P. M.; Riggs, J. B. On-line Optimization of the Tennessee Eastman Challenge Problem, J. Process Control, *10*, pp. 19-33. 2000.

Elliott, T. R.; Luyben, W. L. Capacity-Based Economic Approach for the Quantitative Assessment of Process Controllability during the Conceptual Design Stage, Ind. Eng. Chem. Res., *34*, pp. 3907-3915. 1995.

Elliott. T. R.; Luyben, W. L. Quantitative Assessment of Controllability during the Design of a Ternary System with Two Recycle Streams, Ind. Eng. Chem. Res., *35*, pp. 3470-3479. 1996.

Elliott, T. R.; Luyben, W. L. Application of the Capacity-Based Economic Approach to an Industrial-Scale Process, Ind. Eng. Chem. Res., *36*, pp. 1727-1737. 1997.

Emets, S. V. An Examination of a Modified Hierarchical Design Structure for Chemical Processes. MS Thesis, Chemical Engineering Department, Texas Tech University, 2003. (Available at http://www.che.ttu.edu/classes/che5000/EmetsThesis.pdf, accessed in January 2004.)

Emets, S. V.; Hoo, K. A.; Mann, U. A Modified Hierarchy for Designing Chemical Processes, Ind. Eng. Chem. Res., *45*, pp. 5037-5043. 2006.

Fabro, J. A.; Arruda, L. V. R.; Neves Jr. F.; Startup of a Distillation Column Using Intelligent Control Techniques, Comput. Chem. Eng., *30*, pp. 309-320. 2005.

Feliu, J. A.; Grau, I.; Alos, M. A.; Hernandez, J. J. M. Match Your Process Constraints Using Dynamic Simulation, Chem. Eng. Prog., December, pp. 42-48. 2003.

Fisher, W. R.; Doherty, M. F.; Douglas, J. M. The Interface between Design and Control. 3. Selecting a Set of Controlled Variables, Ind. Eng. Chem. Res., *27*, pp. 611-615. 1988.

Fonyo, Z. Design Modifications and Proper Plantwide Control, Comput. Chem. Eng., *18*, pp. S483-S492. 1994.

Foss, A.S. Critique of Chemical Process Control Theory, AIChE J.,*19* (2), pp. 209-214. 1973.

Garelli, F.; Mantz, R. J.; Battista, H. D. Limiting Interactions in Decentralized Control of MIMO Systems, J. Process Control, *16*, pp. 473-483. 2006.

Georgakis, C.; Uzturk, D.; Subramanian, S.; Vinson, D. R. On the Operability of Continuous Processes, Control Eng. Pract., *11*, pp. 859-869. 2003.

Gilliland, E. R.; Reed, C. E. Degrees of Freedom in Multicomponent Absorption and Rectification Columns, Ind. Eng. Chem., *34*, pp. 551-557. 1942.

Gilliland, E. R.; Goud, L. A.; Boyle, T. J. Dynamic Effects of Material Recycle. In Preprints of Joint Automatic Control Conference, 1964, California, USA, pp. 140-146.

Goel, H. D.; Grievink, J.; Herder, P. M.; Weijnen, M. P. C. Integrating Reliability Optimization into Chemical Process Synthesis, Reliab. Eng. Syst Saf., *78*, pp. 247-258. 2002.

Gonzalez, A. H.; Odloak, D.; Marchetti, J. L. Predictive Control Applied to Heat-Exchanger Networks, Chem. Eng. Process., *45*, pp. 661–671. 2006.

Govind, R.; Powers, G. J. Control System Synthesis Strategies, AIChE J., 28, pp. 60-73. 1982.

Grassi, V. G. Dynamic Simulation as a Tool to Integrate Process Design and Process Control, ISA Trans., *32*, pp. 323-332. 1993.

Groenendijk, A. J.; Dimian, A. C.; Iedema, P. D. Systems Approach for Evaluating Dynamics and Plant-Wide Control of Complex Plants, AIChE J., *46*, pp. 133-145. 2000.

He, M. J.; Cai, W. J. New Criterion for Control-Loop Configuration of Multivariable Processes, Ind. Eng. Chem. Res., *43*, pp. 7057-7064. 2004.

Heath, J. A.; Kookos, I. K.; Perkins, J. D. Process Control Structure Selection based on Economics, AIChE J., *46*, pp. 1998-2016. 2000.

Henry, R. M.; Mujtaba, I. M. Distillation Column Control: The Use of Feed Temperature to Respond to Modest Variations in Feed Composition, Comput. Chem. Eng., *23*, pp. S265-S268. 1999.

Herrmann, G.; Spurgeon, S. K.; Edwards, C. A Model-Based Sliding Mode Control Methodology Applied to the HDA-Plant, J. Process Control, *13*, pp. 129-138. 2003.

Horwitz, B. A.; Nocera, A. J. Are You “Scotomatized” by Your Simulation Software?, Chem. Eng. Prog., September, pp. 68-71. 1996.

Hugo, A. J.; Taylor, P. A.; Wright, J. D. Approximate Dynamic Models for Recycle Systems, Ind. Eng. Chem. Res., *35*, pp. 485-487. 1996.

Jacobsen, E. W. Effect of Recycle on the Plant Zero Dynamics. Comput. Chem. Eng., *21*, pp. S279-S284, 1997.

Jang, W. H.; Hahn, J.; Hall, K. R. Genetic/Quadratic Search Algorithm for Plant Economic Optimizations Using a Process Simulator, Comput. Chem. Eng., *30*, pp. 285-294. 2005.

Jockenhovel, T.; Biegler, L. T.; Wachter, A. Dynamic Optimization of the Tennessee Eastman Process Using The OptControlCentre, Comput. Chem. Eng., *27*, pp. 1513-1531. 2003.

Johns, W. R. Process Synthesis: Poised for a wider role, Chem. Eng. Prog., April, pp. 59-65. 2001.

Jorgensen, J. B.; Jorgensen, S. B. Towards Automatic Decentralized Control Structure Selection, Comput. Chem. Eng., *24*, pp. 841-846. 2000.

Kanadibhotla, R. S.; Riggs, J. B. Nonlinear Model Based Control of a Recycle Reactor Process, Comput. Chem. Eng., *19*, pp. 933-948. 1995.

Kao, Y. K.; Yan, Z. Dynamic Modeling and Simulation of Simple Membrane Permeators, Chem. Eng. Commun., *59*, pp. 343-370. 1987.

Kapoor, N.; McAvoy, T. J.; Marlin, T. E. Effect of Recycle Structure on Distillation Tower Time Constants, AIChE J., 32, pp. 411-418. 1986.

Kassidas, A.; Patry, J.; Marlin, T. Integrating Process and Controller Models for the Design of Self-Optimizing Control, Comput. Chem. Eng., *24*, pp. 2589-2602. 2000.

Keller, G. E.; Bryan, P. F. Process Engineering Moving in New Directions, Chem. Eng. Prog., January, pp. 41-50. 2000.

Kim, Y.; Lee, B.; Eo, S.; Yoon, E. S. A Study on the Evaluation and Improvement of Structural Controllability of Chemical Processes, Comput. Chem. Eng., *24*, pp. 931-936. 2000.

Kocis, G. R.; Grossmann, I. E. A Modeling and Decomposition Strategy for the MINLP Optimization of Process Flowsheets., Comput. Chem. Eng., *13*, pp. 797-819. 1989.

Konda, N. V. S. N. M.; Rangaiah, G. P.; Krishnaswamy, P. R. Systematic Classification of Plant-Wide Control System Design Procedures with Application to the HDA Process, Presented at AIChE Annual Meeting, Nov. 2003, San Francisco, USA.

Konda, N. V. S. N. M.; Rangaiah, G. P.; Krishnaswamy, P. R. Plant-Wide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics, Ind. Eng. Chem. Res., *44*, pp. 8300-8313. 2005.

Konda, N. V. S. N. M.; Rangaiah, G. P.; Krishnaswamy, P. R. A Simple and Effective Procedure for Control Degrees of Freedom, Chem. Eng. Sci., *61*, pp. 1184-1194. 2006.

Konda, N. V. S. N. M.; Rangaiah, G. P.; Lim, D. K. H. Optimal Process Design and Effective Plant-Wide Control of Industrial Processes by Simulation-based Heuristic Approach, Ind. Eng. Chem. Res., *45*, pp. 5955-5970. 2006.

Konda, N. V. S. N. M.; Rangaiah, G. P. Performance Assessment of Plant-Wide Control Systems of Industrial Processes, Ind. Eng. Chem. Res., *46*, pp. 1220-1231. 2007.

Kookos, I. K.; Perkins, J. D. Heuristic-Based Mathematical Programming Framework for Control Structure Selection, Ind. Eng. Chem. Res., *40*, pp. 2079-2088. 2001a.

Kookos, I. K.; Perkins, J. D. An Algorithm for Simultaneous Process Design and Control, Ind. Eng. Chem. Res., *40*, pp. 4079-4088. 2001b.

Kookos, I. K.; Perkins, J. D. An Algorithmic Method for the Selection of Multivariable Process Control Structures, J. Process Control, *12*, pp. 85-99. 2002.

Kumar, A.; Daoutidis, P. Nonlinear Dynamics and Control of Process Systems with Recycle, J. Process Control, *12*, pp. 475-484. 2002.

Kwauk, M. A System for Counting Variables in Separation Processes, AIChE J., *2*, pp. 240-248. 1956.

Laganier, F. Dynamic Process Simulation Trends and Perspectives in an Industrial Context, Comput. Chem. Eng., *20*, pp. S1595-S1600, 1996.

Lakshminarayanan, S.; Takada, H. Empirical Modelling and Control of Processes with Recycle: Some Insights via Case Studies, Chem. Eng. Sci., *56*, pp. 3327-3340. 2001.

Lakshminarayanan, S.; Onodera, K.; Madhukar, G. M. Recycle Effect Index: A Measure to Aid in Control System Design for Recycle Processes, Ind. Eng. Chem. Res., *43*, pp. 1499-1511. 2004.

Larsson, T. Studies on Plantwide Control. Dr.Ing. Thesis, Department of Chemical Engineering, Norwegian University of Science and Technology. 2000.

Larsson, T.; Hesteturn, K.; Hovland, E.; Skogestad, S. Self-Optimizing Control of a Large-Scale Plant: The Tennessee Eastman Process, Ind. Eng. Chem. Res., *40*, pp. 4889-4901. 2001.

Larsson, T.; Govtsmark, M. S.; Skogestad, S.; Yu, C. C. Control Structure Selection for Reactor, Separator, and Recycle Processes, Ind. Eng. Chem. Res., *42*, pp. 1225-1234. 2003.

Lausch, H. R.; Wozny, G.; Wutkewicz, M.; Wendeler. H. Plant-Wide Control of an Industrial Process, Trans. IChemE., *76*, Part A. pp. 185-192. 1998.

Lee, P. L.; Li, H.; Cameron, I. T. Decentralized Control Design for Nonlinear Multi-Unit Plants: A Gap Metric Approach, Chem. Eng. Sci., *55*, pp. 3743-3758. 2000.

Liggin, W. L. UOP Thermal Hydrodealkylation (THDA) Process. In Handbook of Petroleum Refining Processes, ed by Meyers, R. A., pp. 2.23-2.26. New York: McGraw-Hill. 1997.

Longwell, E. J. Dynamic Modeling for Process Control and Operability, ISA Trans., *33*, pp. 3-10. 1994.

Loperena, R. M.; Solar, R.; Ramirez, J. A. Balanced Control Scheme for Reactor/Separator Processes with Material Recycle, Ind. Eng. Chem. Res., *43*, pp. 1853-1862. 2004.

Lu, J. Z. Challenging Control Problems and Emerging Technologies in Enterprise Optimization, Control Eng. Pract., *11*, pp. 847-858. 2003.

Luyben, W. L. Process Modeling, Simulation, and Control for Chemical Engineers. pp. 15-162, New York: McGraw-Hill. 1990.

Luyben, W.L. Dynamics and Control of Recycle Systems. 1. Simple Open-loop and Closed-Loop Systems, Ind. Eng. Chem. Res., *32*, pp. 466-475. 1993.

Luyben, M. L.; Floudas, C. A. Analyzing the Integration of Design and Control – 2. Reactor-Separator-Recycle System, Comput. Chem. Eng., *18*, pp. 971-994. 1994.

Luyben, W. L. Design and Control Degrees of Freedom, Ind. Eng. Chem. Res., 35, pp. 2204-2214. 1996.

Luyben, M. L.; Tyreus, B. D.; Luyben, W. L. Plantwide Control Design Procedure, AIChE J., *43*, pp. 3161-3174. 1997.

Luyben, W. L. External Versus Internal Open-Loop Unstable Processes, Ind. Eng. Chem. Res., *37*, pp. 2713–2720. 1998.

Luyben, W. L.; Tyreus, B. D.; Luyben, M. L. Plantwide Process Control. New York: McGraw-Hill. 1999.

Luyben, W. L. Inherent Dynamic Problems with On-Demand Control Structures, Ind. Eng. Chem. Res., *38*, pp. 2315-2329. 1999.

Luyben, W. L. Control of Outlet Temperature in Adiabatic Tubular Reactors, Ind. Eng. Chem. Res., *39*, pp. 1271-1278. 2000a.

Luyben, W. L. Design and Control of Gas-Phase Reactor/Recycle Processes with Reversible Exothermic Reactions, Ind. Eng. Chem. Res., *39*, pp. 1529-1538. 2000b.

Luyben, W. L. Impact of Reaction Activation Energy on Plant-Wide Control Structures in Adiabatic Tubular Reactor Systems, Ind. Eng. Chem. Res., *39*, pp. 2345-2354. 2000c.

Luyben, W. L. Effect of Design and Kinetic Parameters on the Control of Cooled Tubular Reactor Systems, Ind. Eng. Chem. Res., *40*, pp. 3623-3633. 2001.

Luyben, W. L. Plantwide Dynamic Simulators in Chemical Processing and Control, New York: Marcel Dekker. 2002.

Luyben, W. L.; Hendershot, D. C. Dynamic Disadvantages of Intensification of Inherently Safer Process Design, Ind. Eng. Chem. Res., *43*, pp. 384-396. 2004.

Lyman, P. R.; Georgakis, C. Plantwide Control of the Tennessee Eastman Problem, Comput. Chem. Eng., *19*, pp. 321-331. 1995.

Lyman, P. R.; Luyben, W. L. Method for Assessing the Effect of Design Parameters on Controllability, Ind. Eng. Chem. Res., *35*, pp. 3484-3497. 1996.

Mahajanam, R. V.; Zheng, A. Evaluation of Cost of Dynamic Controllability and Optimal Surge Capacity without Dynamic Models, Ind. Eng. Chem. Res., *41*, pp. 3877-3883. 2002.

Mandler, J. A. Modeling for Control Analysis and Design in Complex Industrial Separation and Liquefaction Processes, J. Process Control, *10*, pp. 167-175. 2000.

Marlin, T. E. Process Control: Designing Processes and Control Systems for Dynamic Performance, Singapore: McGraw-Hill, 1995.

Martinson, W. S.; Barton, P. I. Distributed Models in Plantwide Dynamic Simulators. AIChE J., *47*, pp. 1372-1386. 2001.

Marquardt, W. Dynamic Process Simulation - Recent Progress and Future Challenges, In Proc. of the Fourth International Conference on Chemical Process Control, Feb. 1991, Texas, USA, pp. 131-180.

McAvoy, T. J.; Ye, N. Base Control for the Tennessee Eastman Problem, Comput. Chem. Eng., *18*, pp. 383-413. 1994.

McAvoy, T. J.; Ye, N.; Gang, C. Nonlinear Inferential Parallel Cascade Control, Ind. Eng. Chem. Res., *35*, pp. 130-137. 1996.

McAvoy, T. J. Synthesis of Plantwide Control Systems Using Optimization, Ind. Eng. Chem. Res., *38*, pp. 2984-2994. 1999.

McGuire, J. T. Pumps for Chemical Processing, New York: Marcel Dekker. 1990.

McKetta, J.J. (ed). Encyclopedia of Chemical Processing and Design. pp. 183-235, New York: Marcel Dekker. 1977.

Meadowcroft, T. A.; Stephanopoulos, G.; Brosilow, C. The Modular Multivariable Controller: 1: Steady-State Properties., AIChE J., *38*, pp. 1254-1277. 1992.

Meeuse, F. M.; Grievink, J. Thermodynamic Controllability Assessment in Process Synthesis. In The Integration of Process Design and Control, ed by Seferlis, P. and Georgiadis, M. C., pp. 146-167. Amsterdam: Elsevier. 2004.

Meindersma, G. W. Membrane Permeation and Pressure Swing Adsorption (PSA) for the Production of High Purity Hydrogen. In Effective Industrial Membrane Processes: Benefits and Opportunities, ed by Turner, M. K., pp. 391-400. New York: Elsevier Applied Science. 1991.

Mizsey, P.; Kalmar, I. Effects of Recycle on Control of Chemical Processes, Comput. Chem. Eng., *20*, pp. S883-S888. 1996.

Moore, C. F. Selection of Controlled and Manipulated Variables. In Practical Distillation Control, ed by Luyben, W. L., pp. 413-439. New York: Van Nostrand Reinhold. 1992.

Morari, M.; Arkun, Y.; Stephanopoulos, G. Studies in the Synthesis of Control Structures for Chemical Processes. Part 1: Formulation of the Problem. Process

Decomposition and the Classification of the Control Tasks. Analysis of the Optimizing Control Structures, AIChE J., *26*, pp. 220-232. 1980.

Morud, J.; Skogestad, S. Effects of Recycle on Dynamics and Control of Chemical Processing Plants, Comput. Chem. Eng., *18*, pp. S529-S534. 1994.

Morud, J.; Skogestad, S. Dynamic Behavior of Integrated Plants, J. Process Control, *6*, pp. 145-146. 1996.

Motee, N.; Rodsari, B. S. Optimal Partitioning in Distributed Model Predictive Control. In Proceedings of the American Control Conference, June 2003, Denver, CO.

Mullins, E.; Oldland, R.; Liu, Y. A.; Wang, S.; Sandler, S. I.; Chen, C. C.; Zwolak, M.; Seavey, K. C. Sigma-Profile Database for Using COSMO-Based Thermodynamic Methods, Ind. Eng. Chem. Res., *45*, pp. 4389-4415. 2006.

Nakagawa, T. Industrial Applications of Membranes for Gas Separation in Japan. In Polymeric Gas Separation Membranes, ed by Paul, D. R. and Yampolskii, Y. P., Boca Raton, FL: CRC Press. 1994.

Narraway, L. T.; Perkins, J. D.; Barton, G. W. Interaction between Process Design and Process Control: Economic Analysis of Process Dynamics. J. Process Control, *1*, pp. 243-250. 1991.

Narraway, L. T.; Perkins, J.D. Selection of Process Control Structure Based on Linear Dynamic Economics, Ind. Eng. Chem. Res., *32*, pp. 2681-2692. 1993.

Narraway, N.; Perkins, J.D. Selection of Process Control Structures Based on Economics, Comput. Chem. Eng., *18*, pp. S511-S515. 1994.

Nelson, D. A.; Douglas, J. M. A Systematic Procedure for Retrofitting Chemical Plants to Operate Utilizing Different Reaction Paths, Ind. Eng. Chem. Res., *29*, pp. 819-829. 1990.

Newell, R. B.; Lee, P. L. Applied Process Control: A Case Study. New York: Prentice Hall. 1989.

Ng, C. S.; Stephanopoulos, G. Synthesis of Control Systems for Chemical Plants, Comput. Chem. Eng., *20*, pp. S999-S1004. 1996.

Oh, M.; Pantelides, C. C. A Modeling and Simulation Language for Combined Lumped and Distributed Parameter Systems, Comput. Chem. Eng. *20*, pp. 611-633. 1996.

Papadourakis, A., Doherty, M. F. and Douglas, J.M. Relative Gain Array for Units in Plants with Recycle, Ind. Eng. Chem. Res., *26*, pp.1259-1262. 1987.

Peng, D. Y.; Robinson, D. B. A New Two-Constant Equation of State, Ind. Eng. Chem. Fundam., *15*, pp. 59-64. 1976.

Perkins, J. D.; Walsh, S. P. K. Optimization as a Tool for Design/Control Integration, Comput. Chem. Eng., *20*, pp. 315-323. 1996.

Pham, Q. T. Degrees of Freedom of Equipment and Processes, Chem. Eng. Sci., 49, pp. 2507-2512. 1994.

Phimister, J. R.; Fraga, E. S.; Ponton, J. W. The Synthesis of Multistep Process Plant Configurations, Comput. Chem. Eng., *23*, pp. 315-326. 1999.

Ponton, J. W.; Laing, D. M. A Hierarchical Approach to the Design of Process Control Systems, Trans. IChemE., *17*, pp. 181-188. 1993.

Ponton, J. W. Degrees of Freedom Analysis in Process Control, Chem. Eng. Sci., *49*, pp. 2089-2095. 1994.

Prasad, R.; Shaner, R. L.; Doshi, K. J. Comparison of Membranes with other Gas Separation Technologies. In Polymeric Gas Separation Membranes, ed by Paul, D. R. and Yampolskii, Y. P., pp. 513-614. Boca Raton, FL: CRC Press. 1994.

Price, R. M. and Georgakis. C. Plantwide Regulatory Control Design Procedure Using Tiered Framework, Ind. Eng. Chem. Res., *32*, pp. 2693-2705. 1993.

Price, R. M.; Lyman, P. R.; Georgakis. C. Throughput Manipulation in Plantwide Control Structures, Ind. Eng. Chem. Res., *33*, pp.1197-1207. 1994.

Qiu, Q. F.; Rangaiah, G.P.; Krishnaswamy, P.R. Application of a Plant-Wide Control Design to the HDA Process, Comp. Chem. Eng., *27*, pp. 73-94. 2003.

Reyes, F.; Luyben, W. L. Steady-State and Dynamic Effects of Design Alternatives in Heat-Exchanger/Furnace/Reactor Processes, Ind. Eng. Chem. Res., *39*, pp. 3335-3346. 2000.

Reyes, F.; Luyben, W. L. Design and Control of a Gas-Phase Adiabatic Tubular Reactor Process with Liquid Recycle, Ind. Eng. Chem. Res., *40*, pp. 3762-3774. 2001.

Ricker, N. L. Optimal Steady-State Operation of the Tennessee Eastman Challenge Process, Comput. Chem. Eng., *19*, pp. 949-959. 1995.

Ricker, N. L.; Lee, J. H. Nonlinear Model Predictive Control of the Tennessee Eastman Challenge Process, Comput. Chem. Eng., *19*, pp. 961-981. 1995.

Ricker, N. L. Decentralized Control of The Tennessee Eastman Challenge Problem, J. Process Control, *6*, pp. 205-221. 1996.

Riggs, J. B. Chemical Process Control. Texas: Ferret. 2001.

Riley, K. F.; Hobson, M. P.; Bence, S. J. Mathematical Methods for Physics and Engineering: A Comprehensive Guide. p. 432, Cambridge: Cambridge University Press. 2002.

Robinson. D.; Chen. R.; McAvoy, T.; Schnelle. P. D. An Optimal Control Based Approach to Designing Plantwide Control System Architectures, J. Process Control, *11*, pp. 223-236. 2001.

Rodriguez, M.; Marcos, A. Plantwide Control Design Using an Expert System. In Proceedings of IFAC 15th Triennial World Congress, 2002. Barcelona, Spain.

Rodriguez, M. A New Algorithm to Develop Hybrid Systems, Comput. Chem. Eng., *30*, pp. 260-267. 2005.

Rudd, D. F.; Watson, C. C. Strategy of Process Engineering. New York: Wiley. 1968.

Sakizlis, V.; Perkins, J. D.; Pistikopoulos, E. N. Recent Advances in Optimization-based Simultaneous Process and Control Design, Comput. Chem. Eng., *28*, pp. 2069-2086. 2004.

Samyudia, Y.; Lee, P. L.; Cameron, I. T. Green, M. Control of Multi-Unit Processing Plants – A Systematic Methodology, Comput. Chem. Eng., *20*, pp. S919-S924. 1996.

Scali, C.; Antonelli, R. Performance of Different Regulators for Plants with Recycle, Comput. Chem. Eng., *19*, pp. S409-414. 1995.

Scali, C.; Ferrari, F. Control of Systems with Recycle by means of Compensators, Comput. Chem. Eng., *21*, pp. S267-S272. 1997.

Scali, C.; Ferrari, F. Performance of Control Systems based on Recycle Compensators in Integrated Plants, J. Process Control, *9*, pp. 425-437. 1999.

Schad, R. C. Don't Let Recycle Streams Stymie Your Simulations, Chem. Eng. Prog., December, pp. 68-76. 1994.

Schad, R. C. Make the Most of Process Simulation, Chem. Eng. Prog., January, pp. 21-27. 1998.

Scott, K. Handbook of Industrial Membranes. Oxford, U. K.: Elsevier. 1995.

Seader, J. D.; Henley, E. J. Separation Process Principles. New York: Wiley. 1998.

Seborg, D. E.; Edgar, T. F.; Mellichamp, D. A. Process Dynamics and Control. New Jersey: Wiley. 2004.

Seferlis, P.; Georgiadis, M. C., (eds). The Integration of Process Design and Control. Amsterdam: Elsevier. 2004.

Seider, W. D.; Seader, J. D.; Lewin, D. R. Product and Process Design Principles: Synthesis, Analysis and Evaluation. New York: Wiley. 2004.

Semino, D.; Giuliani, G. Control Configuration Selection in Recycle Systems by Steady State Analysis, Comput. Chem. Eng., *21*, pp. S273–S278. 1997.

Skogestad, S. Plantwide Control: The Search for the Self-Optimizing Control Structure, J. Process Control, *10*, pp. 487-507. 2000a.

Skogestad, S. Self-Optimizing Control: The Missing Link Between Steady-State Optimization and Control, Comput. Chem. Eng., *24*, pp. 569-575. 2000b.

Skogestad, S. Control Structure Design for Complete Chemical Plants. Comput. Chem. Eng., *28*, pp. 219-234. 2004.

Skogestad, S.; Jacobsen, E. W.; Morari, M. Inadequacy of Steady-State Analysis for Feedback Control: Distillate-Bottom Control of Distillation Columns, Ind. Eng. Chem. Res., *29*, pp. 2339-2346. 1990.

Skogestad, S. and Postlethwaite, L. Multivariable feedback control. Wiley: New York. 1996.

Sloley, A. W. Properly Design Thermosyphon Reboilers. Chem. Eng. Prog., *93*, pp. 52-64. 1997.

Smith, B. D. Design of Equilibrium Stage Processes. New York: McGraw-Hill. 1963.

Smith, R. Chemical Process Design. Singapore: McGraw-Hill. 1995.

Sowa, C.J. Make the Move to Dynamic Simulation, Chem. Eng. Prog., August, pp. 44-47. 1997.

Stanley, G.; Galarraga, M.M.; McAvoy, T. J. Shortcut Operability Analysis. 1. The Relative Disturbance Gain, Ind. Eng. Chem. Process Des. Dev., *24*, pp.1181-1188. 1985.

Stephanopoulos, G. Chemical Process Control: An Introduction to Theory and Practice. New Delhi: Prentice Hall. 1984.

Stephanopoulos, G. Synthesis of Control Systems for Chemical Plants: A Challenge for Creativity, Comput. Chem. Eng., *7* (4), pp. 331-365. 1983.

Stephanopoulos, G. and Ng, C. Perspectives on the Synthesis of Plant-Wide Control Structures, J. of Process Control, *10*, pp. 97–111. 2000.

Svrcek, W. Y.; Mahoney, D. P.; Young, B. R. A Real-Time Approach to Process Control. New York: Wiley. 2000.

Taiwo, O. The Design of Robust Control Systems for Plants with Recycle, Int. J. Control, 43, pp. 671-678. 1986.

Taiwo, O.; Krebs, V. Robust Control System Design for Plants with Recycle, Chem. Eng. J., *61*, pp. 1-6. 1996.

Tian, Z.; Hoo, K. A. Multiple Model-Based Control of the Tennessee-Eastman Process, Ind. Eng. Chem. Res., *44*, pp. 3187-3202. 2003.

Tremblay, E.; Desbiens, A.; Pomeleau, A. Control of a Process with Recycle: Robustness of a Recycle Compensator, Ind. Eng. Chem. Res., *45*, pp. 1924-1934. 2006.

Tu, H.; Rinard, I. ForeSee – A Hierarchical Dynamic Modeling and Simulation System of Complex Processes, Comput. Chem. Eng., *30*, pp. 1324-1345. 2006.

Turkay, M.; Gurkan, T.; Ozgen, C. Synthesis of Regulatory Control Structures for a Styrene Plant, Comput. Chem. Eng., *17*, pp. 601-608. 1993.

Turton, R.; Bailie, R. C.; Whiting, W. B.; Shaeiwitz, J. A. Analysis, Synthesis, and Design of Chemical Processes. Englewood Cliffs, NJ: Prentice Hall. 2003.

Tyreus, B. D. Object Oriented Simulation. In Practical Distillation Control, ed by Luyben, W. L., pp. 72-85. New York: Van Nostrand Reinhold. 1992.

Umeda, T.; Kuriyama, T.; Ichidawa, A. A Logical Structure for Process Control System Synthesis. In Proceedings of IFAC Congress, 1978. Helsinki.

Umeda, T.; Kuriyama, T.; Kobayashi, S.; Ichikawa, A. Interactive Solution to Multiple Criteria Problems in Chemical Process Design, Comput. Chem. Eng., *4*, pp. 157-165. 1980.

Vadigepalli, R. and Doyle III, F. J. Structural Analysis of Large-Scale Systems for Distributed State Estimation and Control Applications, Control Eng. Pract., 11, pp. 895-905. 2003.

Vasbinder, E. M.; Hoo, K. A. Decision-Based Approach to Plantwide Control Structure Synthesis, Ind. Eng. Chem. Res., *42*, pp. 4586-4598. 2003.

Vasbinder, E. M.; Hoo, K. A.; Mann, U. Synthesis of Plantwide Control Structures using a Decision-Based Methodology. In The Integration of Process Design and Control, ed by Seferlis, P. and Georgiadis, M.C., pp. 375-400. Amsterdam: Elsevier, 2004.

Wang, P.; McAvoy, T. J. Synthesis of Plantwide Control Systems Using a Dynamic Model and Optimization, Ind. Eng. Chem. Res., *40*, pp. 5732-5742. 2001.

Ward, J. D.; Mellichamp, D. A.; Doherty, M. F. Importance of Process Chemistry in Selecting the Operating Policy for Plants with Recycle, Ind. Eng. Chem. Res., *43*, pp. 3957-3971. 2004.

Ward, J. D.; Mellichamp, D. A.; Doherty, M. F. Novel Reactor and Recycle Rate Policies for Optimal Process Operation in the Plantwide Context, Ind. Eng. Chem. Res., *44*, pp. 6729-6740. 2005.

Ward, J. D.; Mellichamp, D. A.; Doherty, M. F. Insight from Economically Optimal Steady-State Operating Policies for Dynamic Plantwide Control, Ind. Eng. Chem. Res., *45*, pp. 1343-1353. 2006.

Watson, D. R.; Dzirbik, D.; Rudolph, J.; Joglekar, G. S. The Integration of Process Simulation in Operational Analysis, Comput. Chem. Eng., *24*, pp. 607-612. 2000.

Williams, D. F. Evaluation of Candidate Salts for Use as High Temperature Heat Transfer Agents. Presented at the AIChE Annual Meeting, 2005, Cincinnati, OH.

Woods, D. R. Process Design and Engineering Practice. New Jersey: PTR Prentice Hall. 1995.

Wu, K. L.; Yu, C. C. Reactor/Separator Processes with Recycle - 1. Candidate Control Structure for Operability, Comput. Chem. Eng., *20*, pp. 1291-1316. 1996.

Wu, K. L.; Yu, C. C. Operability for Processes with Recycles: Interaction between Design and Operation with Application to the Tennessee Eastman Challenge Process, Ind. Eng. Chem. Res., *36*, pp. 2239-2351. 1997.

Ye, N.; Mc Avoy, T.; Kosanovich, K.; Piovoso, M. Optimal Averaging Level Control for the Tennessee Eastman Problem, Can. J. Chem. Eng., *73*, pp. 234-240. 1995.

Yi, C. K.; Luyben, W. L. Evaluation of Plant-Wide Control Structures by Steady-State Disturbance Sensitivity Analysis, Ind. Eng. Chem. Res., *34*, pp. 2393-2405. 1995.

Yu, C. C. Autotuning of PID Controllers: Relay Feedback Approach. New York: Springer. 1999.

Zheng, A.; Mahajanam, R. V. A Qualitative Controllability Index, Ind. Eng. Chem. Res., *38*, pp. 999-1006. 1999.

Zheng, A.; Mahajanam, V.; Douglas, J. M. Hierarchical Procedure for Plantwide Control System Synthesis, AIChE J., *45*, pp. 1255-1265. 1999.

Zhu, G. Y.; Henson, M. A.; Ogunnaike, B. A. A Hybrid Model Predictive Control Strategy for Nonlinear Plant-Wide Control, J. Process Control, *10*, pp. 449-458. 2000.

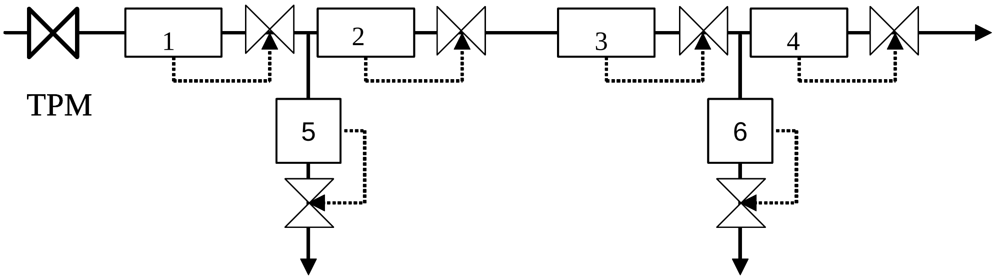
Zhu, G. Y.; Henson, M. A. Model Predictive Control of Interconnected Linear and Nonlinear Processes, Ind. Eng. Chem. Res., *41*, pp. 801-816. 2002.

Zolandz, R. R.; Fleming, G. K. Economics. In Membrane Handbook, ed by Winston, W. S. and Sirkar, K. K., New York: Chapman and Hall. 1992.

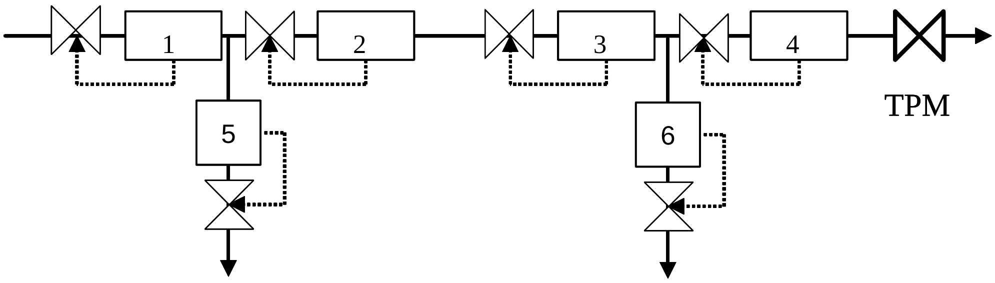
APPENDIX A

Self-Consistency for Inventory Control

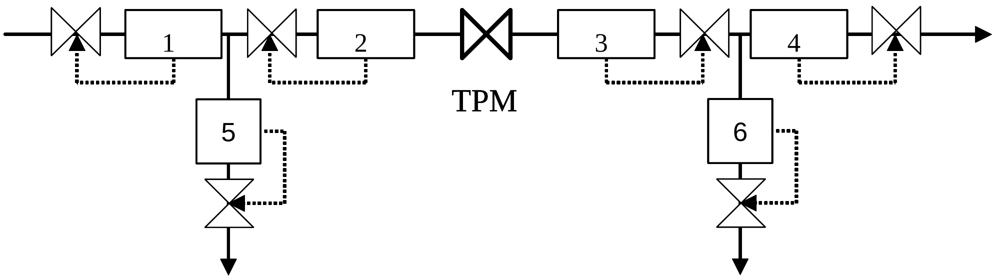
Price and Georgakis (1993) defined three self-consistent inventory control structures based on throughput manipulator (TPM) decision. If the flow control on the feed is selected as the TPM (alternative 1), the inventory should be controlled in the direction of flow. On the other hand, if TPM is the flow control over the product stream (alternative 2), the inventory should be controlled in the direction opposite to flow. If the TPM is other than these two choices, the inventory should be controlled as shown in alternative 3 where the TPM is an internal/implicit variable such as reactor temperature. The inventory in the side chains should be controlled in such a way that the disturbance propagation is away from the primary process path (Figure A.1). Price and Georgakis (1993) proved that these self-consistent structures are superior to self-inconsistent structures in terms of performance as they have better disturbance attenuation capability. Hence, the concept of self-consistency is very useful in the design and analysis of PWC systems.



Alternative 1. Fixed Feed Flow Control



Alternative 2. On-Demand Product Control



Alternative 3. Internal/Implicit Manipulator for Throughput

Figure A.1: Alternative Configurations for Throughput Manipulator. Blocks 1 to 6 represent units with inventory

APPENDIX B

Application of CDOF Procedure to Integrated Processes

The proposed procedure is applied to several other flowsheets (Figures B.1 to B.3) to further validate its applicability. The reactor in these figures is assumed to be CSTR. The CDOFs are compared with those in the literature (Table B.1). It is observed that the proposed procedure is capable of computing the CDOF correctly even for highly integrated processes.

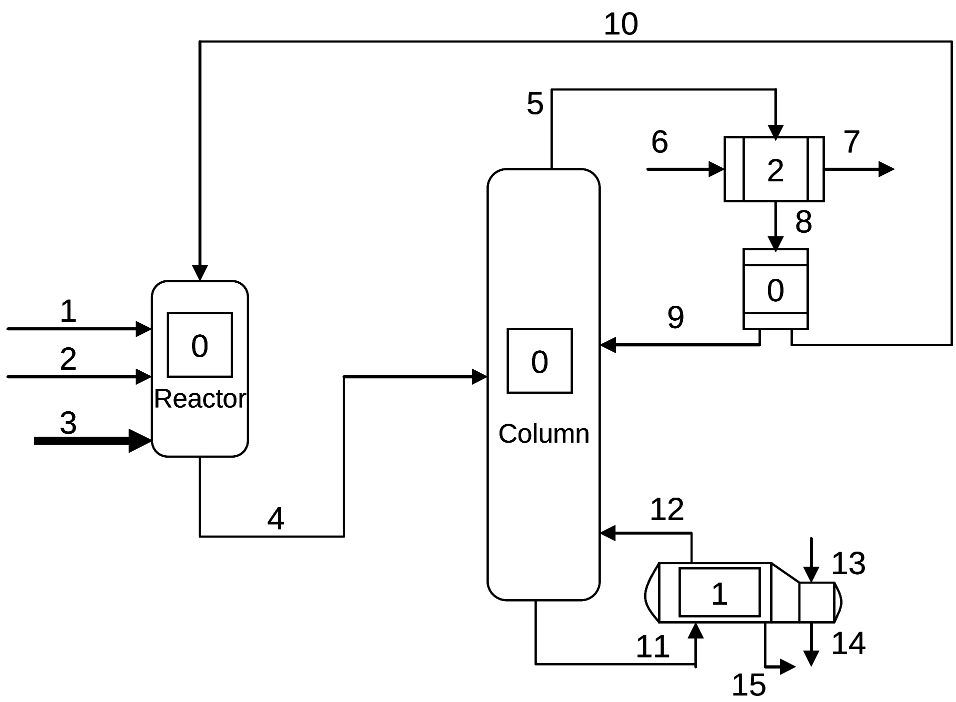


Figure B.1: Reactor/Column Ternary Process with One Recycle (Luyben, 1996)

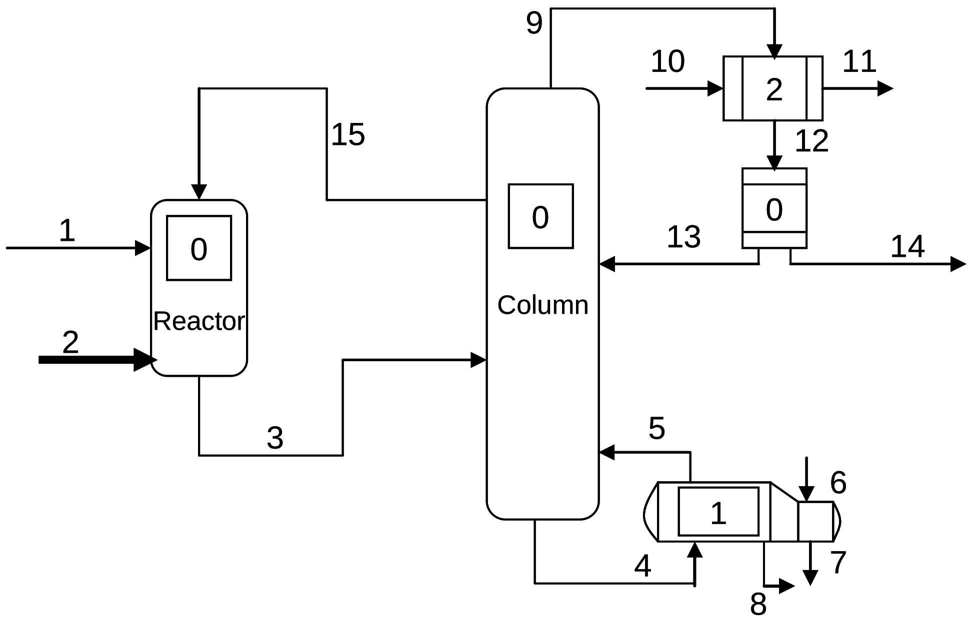


Figure B.2: Reactor/Side Stream Column Process (Luyben, 1996)

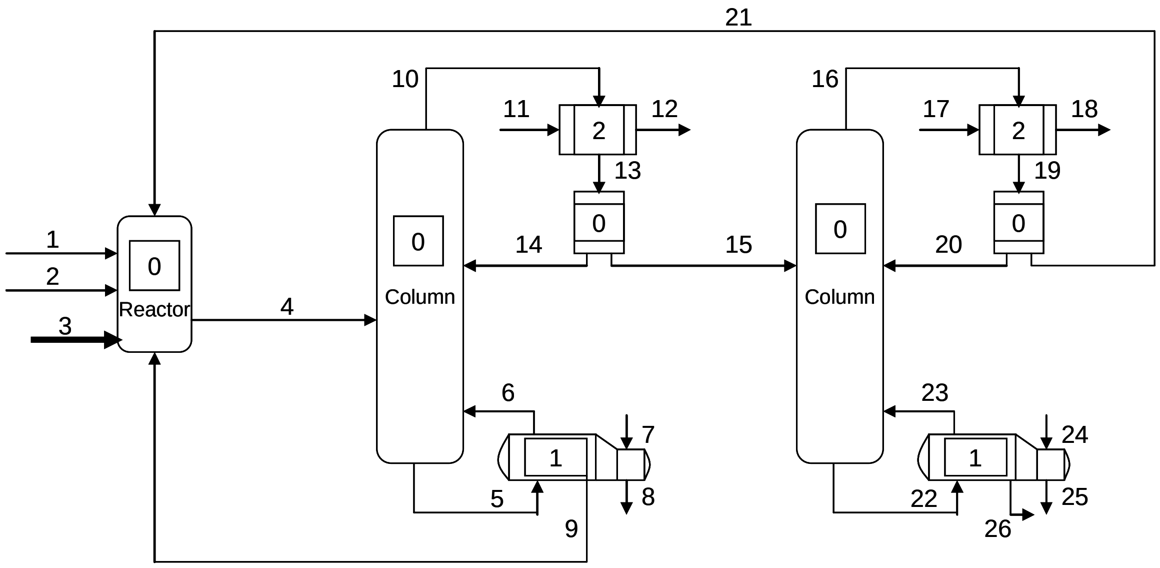


Figure B.3: Reactor/Two-Column Ternary Process with Two Recycles (Luyben, 1996)

Table B.1: CDOF for Processes shown in Figures B.1 to B.3

Figure Number	CDOF from equation 9 and the concept of redundancy	Total CDOF from Luyben (1996)
B.1	9 [= 15 - (2+1+1×3)]	9
B.2	9 [= 15 - (2+1+1×3)]	9
B.3	14 [= 26 - (2+1+2+1+2×3)]	14

APPENDIX C

Resulting Control Structure for Alternative 4 after Step 6 of Proposed PWC Methodology and Controller Parameters for Alternative 7

Proposed integrated framework is applied to alternative 4 and the resulting control structure (after step 6 of the procedure) is given in Table C.1. Tuning parameters for Alternative 7 are given in Table C.2. Flow, pressure and level controllers are tuned according to Luyben's (2002) guidelines. Flow controllers are PI type with a gain of 0.5 and reset time of 0.25 min. Pressure controllers are of the PI type, with a gain of 2 and reset time 10 min. In general, all level controllers are P-only type with a proportional gain of either 5 or 10. PI controllers are used for temperature control, and are tuned using the auto-tuning method with a sensor span of 200 ^{0}F. Composition controllers are also of the PI type and auto-tuning is used to generate initial values for the controller parameters. If necessary, these controllers are then fine-tuned to give reasonably good and robust performance, even for the worst-case disturbance.

Table C.1: Resulting Control Structure for Alternative 4 after step 6 of the Proposed PWC Methodology (Konda et al. 2005)

No	Process Variable	Controller Output
1	Flash level	Stabilizer feed flow rate
2	Stabilizer reboiler level	Stabilizer bottoms flow rate
3	Stabilizer condenser level	Stabilizer condenser duty
4	Stabilizer condenser pressure	Stabilizer overhead flow
5	Product column condenser level	Product column reflux flow
6	Product column reboiler level	Product column bottoms flow
7	Product column condenser pressure	Product column condenser duty
8	Flash pressure	Flash vapor flow
9	Toluene feed flow	Toluene feed valve
10	Hydrogen to aromatics ratio at the reactor inlet	Hydrogen feed flow rate
11	Stabilizer bottoms purity	Stabilizer reboiler duty
12	Product column bottoms purity	Product column reboiler duty
13	Stabilizer overhead purity	Stabilizer reflux flow
14	Product column overhead purity	Product column overhead flow
15	Reactor effluent temperature after quench	A part of the flash drum liquid flow rate
16	Flash temperature	Cooler duty
17	Recycle column condenser level	Toluene recycle flow rate
18	Recycle column reboiler level	Recycle reboiler vapor flow rate
19	Recycle column condenser pressure	Recycle column condenser duty
20	Recycle column ovhd purity	Recycle column reflux flow rate
21	Recycle column bottoms purity	Recycle column bottoms flow
22	Reactor inlet temperature	Furnace duty

Table C.2: Controller Parameters for Alternative 7

No	Controller	Tuning Parameters	
		K_c (%/%)	τ_i (Min)
1	Flash level controller	10	-
2	Stabilizer reboiler level controller	5	-
3	Stabilizer condenser level controller	5	-
4	Product column reboiler level controller	5	-
5	Product column condenser level controller	5	-
6	Flash pressure controller	2	2
7	Stabilizer condenser pressure controller	2	10
8	Product column condenser pressure controller	2	10
9	Toluene feed flow controller	0.5	0.25
10	Hydrogen to aromatics ratio controller	0.5	0.25
11	Permeate flow controller	0.5	0.25
12	Toluene split controller	0.5	0.25
13	Stabilizer bottoms temperature controller	2.41	1.21
14	Product column bottoms temperature controller	9.26	1.33
15	Stabilizer overhead purity controller	0.14	11.0
16	Product column overhead controller	1.13	11.6
17	1st reactor inlet temperature controller	1.58	0.18
18	2nd reactor inlet temperature controller	0.54	0.18
19	Flash temperature controller	0.07	0.29

APPENDIX D

Steady-State Simulation Models of Ethylene Glycol and Propylene Glycol Processes

As shown in Figure D.1, ethylene glycol (EG) is produced from the raw materials ethylene-oxide (EO) and water. The reactor is modeled as a CSTR in which the reaction (ethylene + water → ethylene glycol) takes place. Mixture of the product and unconverted raw materials are then separated in a distillation column. Distillation column has 10 trays and the feed is introduced at the 5th tray. Unconverted raw materials are recovered as distillate and recycled to the reactor, while the product (EG) is recovered from the bottom.

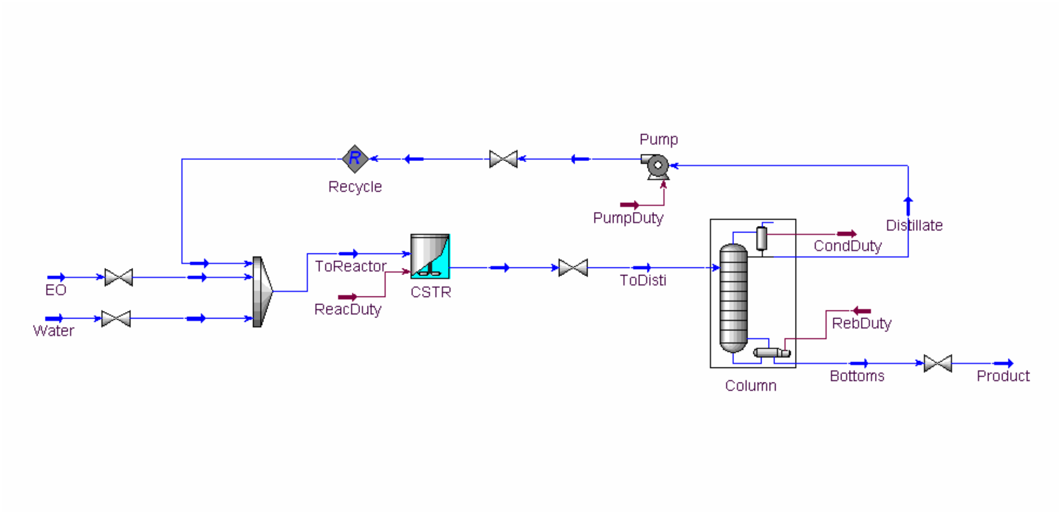


Figure D.1: Steady-State Simulation Model of Ethylene Glycol Process

As shown in Figure D.2, propylene glycol (PG) is manufactured from propylene-oxide (PO) and water. Reactor is modeled as a CSTR. Unconverted raw materials and product are then sent to a distillation column. Pure PG is recovered at the bottom of the column and unconverted raw materials are recovered in the distillate. Distillate is then recycled to reactor section.

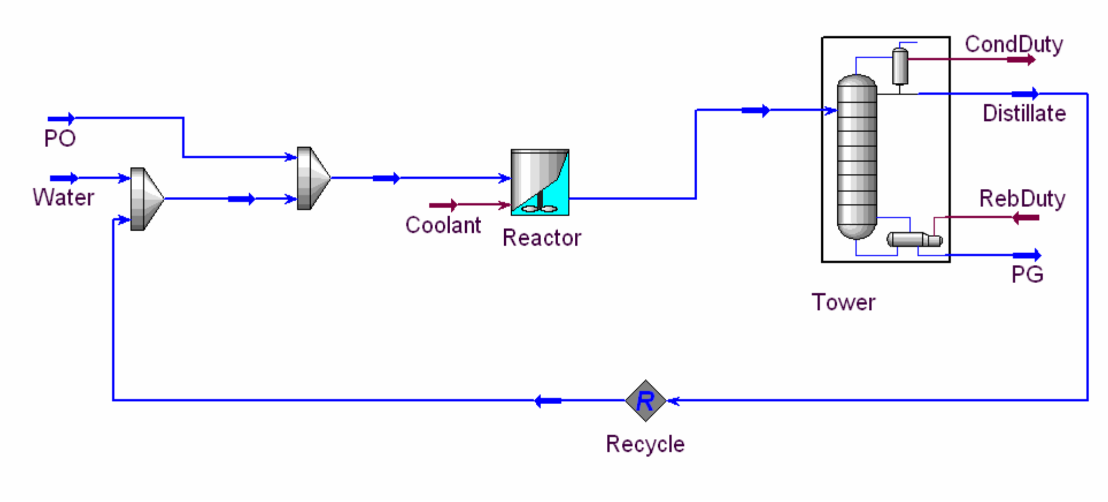


Figure D.2: Steady-State Simulation Model of Propylene Glycol Process

Appendix E
CV OF THE AUTHOR

EDUCATION

National University of Singapore, Singapore 2002-2006
Doctor of Philosophy (Chem. Engg.) - CAP: 4.38/5.00
National Institute of Technology, Warangal, India 1998-2002
Bachelor of Technology (Chem. Engg.) - First Class with Distinction

EXPERIENCE

Doctoral Research, NUS

- Optimal design of petrochemical processes
- Design of equipments and heat exchanger networks
- Synthesis of regulatory control systems for integrated processes

Co-curricular Activities, NUS

- Tutor : Process Design
- Mentor : UG Research Projects
- Demonstrator : Unit Operations Laboratory

Bachelors, NITW

- Industrial Training : Godavari Fertilizers & Chemicals Ltd., India
- Design Project : Manufacture of Poly Vinyl Chloride
- Research Project : Modeling of Fluidized Bed Bioreactor

HONOURS & AWARDS

- Best Tutor, fall 2005
- 3rd Best Poster, Graduate Student Symposium, ChBE, NUS, 2005
- Graduate Research Scholarship, NUS (July 2002 – July 2006)
- Top 0.4% out of 100,000 students in EAMCET (A state level technical examination, Andhra Pradesh), India, 1998

PUBLICATIONS

1. Konda, N.V.S.N.M.; Rangaiah, G.P.; Krishnaswamy, P.R. Plant-Wide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics, *Ind. Eng. Chem. Res.*, 44, 8300-8313, 2005.
2. Konda, N.V.S.N.M.; Rangaiah, G.P.; Krishnaswamy, P.R. A Simple and Effective Procedure for Control Degrees of Freedom, *Chem. Eng. Sci*., 61, 1184-1194, 2006.
3. Konda, N.V.S.N.M.; Rangaiah, G.P.; Lim, D.K.H. Optimal Process Design and Effective Plant-Wide Control of Industrial Processes by Simulation-based Heuristic Approach, *Ind. Eng. Chem. Res.*, 45, 5955-5970. 2006.
4. Lim, D.K.H.; Konda, N.V.S.N.M.; Rangaiah, G.P. Synthesis and Design of Chemical Processes, *Journal of The Institution of Engineers*, Singapore, 45, 39-49, 2005.

5. Konda, N.V.S.N.M.; Rangaiah, G.P. Performance Assessment of Plant-Wide Control Systems of Industrial Processes, *Ind. Eng. Chem. Res.*, 46, 1220-1231. 2007.

6. Zhigui, G.; Konda, N.V.S.N. M.; Rangaiah, G.P. Simulation and Optimization of a Vinyl Chloride Monomer Plant, submitted to *Journal of The Institution of Engineers*, Singapore, June 2006.

PRESENTATIONS

1. Konda, N.V.S.N.M.; Rangaiah, G. P. Performance Assessment of Plant-Wide Control Systems of Industrial Processes, *11th APCCHE Congress*, Kuala Lumpur, Malaysia, August, 2006.

2. Konda, N.V.S.N.M.; Rangaiah, G. P.; Krishnaswamy, P. R. Optimal Plant-Wide Design and Control of Industrial Processes, *2nd Annual Graduate Student Symposium*, NUS, Singapore, 2005.

3. Konda, N.V.S.N.M.; Rangaiah, G. P.; Krishnaswamy, P. R. Simulation based Heuristics Methodology for Plant-Wide Control of Industrial Processes, *16th IFAC World Congress,* Prague, Czech Republic, 2005.

4. Konda, N.V.S.N.M.; Rangaiah, G. P.; Krishnaswamy, P. R. A Simple and Effective Procedure for Control Degrees of Freedom, *7th World Congress of Chemical Engineers,* Glasgow, Scotland, 2005.

5. Konda, N.V.S.N.M.; Rangaiah, G. P.; Krishnaswamy, P. R. Plant-Wide Control of Industrial Processes: An Integrated Framework of Simulation and Heuristics, *1st Annual Graduate Student Symposium*, NUS, 2004.

6. Konda, N.V.S.N.M.; Rangaiah, G. P.; Krishnaswamy, P. R. Systematic Classification of Plant-Wide Control System Design Procedures with Application to the HDA Process, *AIChE Annual Meeting,* San Francisco, USA, 2003.

TECHNICAL TALKS

Basics of Distillation: Design & Simulation, ChBE, NUS, March 2005
Introduction and Overview of HYSYS, ChBE, NUS, March 2004

EXTRA CURRICULAR ACTIVITIES

- General Secretary
  Graduate Students' Association - ChBE, NUS, 2003 - 2005
- Executive member of Technical Committee
  Graduate Student Symposium, ChBE, NUS, 2004 & 2005
- Executive member of Organizing Committee
  CHEMELIXIR (National Level Symposium), NITW, 2002
- Member of AIChE (2003 – 2004) & IICh