FEASIBILITY AND OPERABILITY ANALYSIS OF

CHEMICAL PROCESS ALTERNATIVES

By

USHA GOLLAPALLI

Bachelor of Technology

Andhra University

Visakhapatnam, India

1997

Submitted to the Faculty of the
Graduate college of the
Oklahoma State University
In partial fulfillment of
the requirements for
the Degree of
MASTER OF SCIENCE
December, 1999

FEASIBILITY AND OPERABILITY ANALYSIS OF

CHEMICAL PROCESS ALTERNATIVES

Thesis Approved:

Karen A. High

Thesis Advisor

Martin S. High

Arland H. Johannes

Wayne B. Powell

Dean of the Graduate College

ACKNOWLEDGEMENTS

It gives me immense happiness and satisfaction to thank all the people who helped me in finishing my Masters successfully. First, I would like to thank my advisor, Dr. Karen High. Her easy going nature and her effort to provide me with financial assistance throughout my Masters has helped in many ways and in many crucial moments of my life in Stillwater. Also, I would like to thank the Environmental Institute for the financial support that they offered for my research.

I would also like to thank my other committee members, Dr. Marty High and Dr. Arland Johannes. Dr. Marty with his encouraging words and ready smile had always been a big help to me. I sincerely appreciate the vast patience that Dr. AJ showed towards me, despite me pestering him constantly for every tiny technical problem that I had. My special thanks to Dr. Rhinehart for his unhesitating help and constant guidance through out my thesis work and to Dr. Whiteley for his advice and suggestions. I would like to convey my gratitude to Mauricio, whose valuable advice helped me a lot in my work. I also thank the industrialists whose responses to my questionnaire gave a sharper focus to this research.

Besides all the technical help that I got, a lot of moral support that I have received from many people has gone a long way in making my school life in Stillwater a memorable and learning experience. Whom can I think of first when I think of Stillwater

than my roommates, Anupama, Durga, Uma and Pratima. The laughter, the fun, the arguments and also the squabbles that I had with them have taught me a lot. The list would be very incomplete if I do not mention my colleague and friend, Rob Wade, who has been an immense support and help throughout my Masters. I would also like to thank Anand, Prashant and Talee.

My more lasting memories in Stillwater are due to Rustom, from whom I probably have learnt the most. Janardhan, my dear friend, is one person who had been with me through all the hills and valleys that I had to traverse before reaching this point. Thank you very much for everything, Jana.

I am lost for words when it comes to my family. My Grand parents, Father, Mother, Sister and all others with their constant encouragement, concern about my welfare, and inexhaustible love and support have made me what I am today. I shall strive my best to stand up to their expectations.

TABLE OF CONTENTS

Chapter Page

LIST OF TABLES

LIST OF FIGURES

NOMENCLATURE

Roman Letters

A	Reciprocal matrix
A_f	Annual worth factor
a_{jk}	numerical equivalent of comparison between criteria j and k
d	Design variable
D	Depreciation factor
E	Environmental Impact
e_{max}	Largest eigenvalue
$f(\,)$	Feasible operating region
F	Flow rate (kg/hr)
F_1	General Process Hazards Factor
F_2	Special Process Hazards Factor
F_d	Depreciable investment
$FEED$	Feed flow rate (kg/hr)
f_I	Inflation factor
$FLSP$	Flash chamber pressure (Pa)
$g(\,)$	Set of inequality constraints
$G(s)$	Transfer function matrix

$h( )$	Set of equality constraints
$HEAT$	Heat duty to the flash chamber (J/s)
i_f	Annual inflation rate
i_r	Interest rate
$j( )$	Capacity constraints
$\boldsymbol{K}$	Steady state gain matrix
$m_{j,I}$	Mass fraction of component j in waste stream I
MO	Multi-Objective function
n	Number of years (yr)
N_y	Project life time (yr)
P	Total mass of product obtained (kg/hr)
P_l	Probability of being in an active state
$PROD$	Product (Methyl Chloride) flow rate (kg/hr)
Q	Quality of control (s)
r	Ratio
s	Controller gain
T	Temperature (^{o}R)
T_x	Tax rate
w_f	Weighing factor
w_i	Flow rate of waste stream, i (kg/hr)
x	State variable
X	Mole fraction
Z_{ij}	Positive score for alternative i with respect to jth criterion

Greek letters

α_x	Weighting factor placed on impact x
Δ	Deviation from optimum value
δ	Change in uncertain parameter
κ_d	Plant disturbance condition number
λ	Failure rate of equipment
μ	Repair rate of equipment
ϕ	Environmental impact index of chemical j (EIU/kg)
σ	Singular values of the gain matrix
θ	Uncertain parameter
$\psi_{i.l,x}$	Specific environmental impact of type x
τ	Period of oscillation (s^{-1})

Subscripts

C	Cold water
D	Deviation from optimum value
H	Hot Water
i	Inflow
M	Mixture
o	Outflow
O	Optimum Value
R	Range

Symbols

$	Economic Feasibility

Abbreviations

AEP	Annual Equivalent Profit
AHP	Analytic Hierarchy Process
C	Controllability
CF	Cash flow
CN	Condition Number
CSTR	Continuous Stirred Tank Reactor
CV	Controlled Variables
DC	Disturbance Cost
DCN	Disturbance Condition Number
DOF	Degrees of Freedom
DV	Disturbance Variables
EIU	Environmental Impact Units
E(SF)	Expected Stochastic Flexibility
F	Flexibility
FI	Flexibility Index
F&EI	Fire and Explosion Index
F&O	Feasibility and Operability
HAZOP	Hazard and Operability Study
HV	Hazard Value

MF	Material Factor
MINLP	Mixed Integer Non Linear Programming
MOO	Multi-Objective Optimization
MV	Manipulated Variables
NPV	Net Present Value
O	Operability
OSHA	Occupational Safety and Health Administration
PFR	Plug Flow Reactor
R	Resiliency
RGA	Relative Gain Array
S	Safety
SF	Stochastic Flexibility
SVA	Singular Value Analysis

Chapter 1

INTRODUCTION

"Environmental Consciousness" has become widely prevalent over the past few years. As the concept of environmentally friendly processes became popular, chemical process industries became concerned with two factors: 1) Their processes should suit the standards set by the environmental organizations like EPA and the laws enforced by the government. 2) Keep the process as lucrative as possible. This lead to the concept of incorporating "green chemistry" into the designs of chemical processes, whose main purpose was to serve in reducing the pollution caused by the processes. Now, the question is:

Will new or altered processes that implement green chemistries and technologies be profitable and operable?

1.1 Introduction to Feasibility & Operability of Chemical Processes

Feasibility and Operability (F&O) of a chemical process refers to the potential of the process to get accepted and be functional in industry. The feasibility and operability of a chemical process is governed by several factors. Some of them are:

- Profitability ($): The revenue generated by the process should be substantial and should be sustained over a period of time, say a year.

- Environmental Impact (E): The impact of the process on the environment should not be hazardous, or in other words any effluents that are generated from the process should not cause any pollution to the surrounding environment.
- Controllability (C): The plant should be capable of rejecting any disturbances upsetting the system and still meet with the set points.
- Resiliency (R): The plant should be capable of tolerating and recovering from undesirable changes and upsets (Grossmann and Morari, 1983).
- Flexibility (F): The plant should be able to operate over a range of conditions while satisfying performance specifications (Swaney and Grossmann, 1985a).
- Safety (S): The operation of the plant should be safe for the people working in the plant and for the surrounding community,

and, more.

All these features can be grouped under one common term, ***Feasibility & Operability***. The first two features, profitability and environmental impact, determine whether the process is acceptable to industry or not. They are grouped under the common term, feasibility. The rest four features determine whether the process can function in industry or not, and are together coined as operability. Operability[1] of an industrial process, in simple words, can be described as the ability of the process to perform satisfactorily in all aspects. The first factor (profitability) is what the industries have their eyes on while choosing between alternative designs, but an unbiased view is that the economics of any

[1] This definition of operability refers in particular to that trait of a plant, which satisfies all the criteria listed above, and more when more criteria are added to the list (See Chapter 8). The definition for operability has varied from author to author in that each defines the term with respect to a different set of criteria (Grossmann and Halemane, 1982; Grossmann et al., 1983b; Grossmann and Morari, 1983a; Palazoglu et al., 1985b; Arkun, 1986; Linnhoff and Kotjabasakis, 1986; Palazoglu and Arkun, 1986; McAvoy, 1987; Palazoglu and Arkun, 1987; Fisher et al., 1988a, b, c; Vijuk and Bruschi, 1988; Goyal, 1993; Thomaidis

industrial process is greatly controlled by the last five. When the process meets with the F&O criteria, it will certainly incur expenses but will ultimately make more money. If the process is environmentally safe, the industry saves on expenses involved in the disposal of wastes or in paying any fines on violation of environmental laws. Lack of controllability, resiliency, flexibility and safety will shut down production itself. So, in other words, regardless of the profit gained by the company over a short period of time, if the chemical process does not satisfy any of the F&O criteria, maintaining these profits over a long term will not be possible and will ultimately lead the company to losses. Hence, the judicial way to make production most economical is to consider all six criteria together and work towards achieving the best of all.

Thus, the main objective of this work is to select the best *feasible* and *operable* design from among a set of alternative designs. To achieve this objective the steps to be followed are:

- Find all criteria that are responsible for making a chemical process design acceptable and functional for industrial operations.
- Develop or suggest quantitative measures to evaluate these criteria.
- Develop simple tools in Aspen Plus™ to evaluate the operability criteria.
- Compare alternative process designs based on these criteria using the tools developed.
- Collaborate with industry to improve and expand the list of criteria.

Before, the aforementioned steps are discussed in detail, the significance of each criterion is described in the following sections.

---

and Pistikopoulos, 1994; Downs and Ogunnaike, 1995; Rovaglio et al., 1995; Pumps, 1996; Eliceche et al., 1998; Schijndel and Pistikopoulos, 1999; Tyreus and Luyben, 1999).

1.1.1 Environmental Impact

There has been an increased focus on the protection of environment in the recent past. Government has passed many stringent environmental laws, which enforce the reduction of pollutant disposal to the environment. Companies are faced with a situation where they have to strictly follow these laws and also work to obtain profits. Compliance with the environmental laws leads to two immediate concerns: 1) First, it increases the amount of work for the companies with the burden of monitoring waste minimization and pollution control in addition to normal operations. 2) Second, the equipment set up to control waste generation and reduce pollutant disposal, their maintenance etc. will increase the costs incurred by the company. A lot of research has been sought to reduce pollution (See Section 2.1.1). The most favored approach is source reduction, in which minimization of waste is attempted where the waste is created. This would prevent waste generation and obviate the need to dispose of undesired chemicals in an environmentally safe manner.

1.1.2 Controllability Analysis

The function of a chemical processing industry is to operate a chemical process by the combination of several units such that the operation leads to the conversion of raw materials into products by any chemical or physical means. The basic principles guiding the operation of the processing units of the chemical process are based on the following objectives (Ogunnaike and Ray, 1994):

- Safe operation of the processing units is desired.

  This means that no unit should be operated at or near conditions considered to be potentially dangerous to the human operators or the equipment or to the environment.

- Specified production rates must be maintained.

  The amount of product output required of a plant at any time is dictated by the market requirements. Thus, production rate specifications must be met and maintained as much as possible.

- Product quality specifications must be maintained.

  Products not meeting with the product quality specifications should be discarded as waste or reprocessed at an additional cost. The need for economic utilization of resources therefore provides the motivation for striving to satisfy product quality specifications.

The operation of any chemical process depends to a great extent on the satisfaction of the above objectives. The task of satisfying these objectives is the function of a control system. The process control system is the entity that is charged with the responsibility for monitoring outputs, making decisions about how best to manipulate inputs so as to obtain desired output behavior, and efficiently implementing such decisions on the process (Ogunnaike and Ray, 1994). If the chemical process deviates from the desired behavior, alterations are made by the control system such that the output is satisfying.

Controllability analysis is nothing but this systematic study of a chemical process at the design stage, evaluating its controllability, and if the process is not controllable suggest ways to restore controllability. Currently, the most striking flaw in any industrial operation is the lack of associative interaction between process design and process control. An improper interaction between the two not only leads to a design which might be uncontrollable, and hence infeasible, but also incurs a lot of expenses while attempting to operate in the uncontrollable regions. This research involves designing and choosing the best control strategy which will improve the performance of the chemical process, from among a set of alternative strategies and also which can be incorporated into the process design, thus leading to a proper interaction between the two.

Two case studies have been examined to validate the methodologies developed for \$, E and C. The first one is a hot and cold water mixing system. This is a very simple system and was used as a base for the development and coding of the singular value analysis. SVA was coded in ASPEN PLUS™, version 9.2. The second case study is the manufacture of methyl chloride by the hydrochlorination of methanol. This chemistry (hydrochlorination of methanol) was selected as it is the commercial mode of production (CMR, 1997), and also this chemistry has been proven to be better in waste minimization, as opposed to thermal chlorination of methane (Dantus, 1995). The appropriate thing to do for this research is to validate the statement that the environmentally friendly nature of a process does not guarantee its operability against a proven environmentally friendly process. For this reason, the second case study has been chosen.

The code developed for singular value analysis for the hot and cold water system is implemented for the methyl chloride process, after making suitable changes to adapt the code to the new system. Three alternate designs were examined, the difference in the designs being the reactors used. Alternate 1 used an adiabatic PFR, alternate 2, an isothermal PFR and alternate 3 used a CSTR. The analysis helped compare the three designs in terms of their profitability, environmental impact and controllability.

1.1.3 Flexibility and Resiliency Analyses

Another important issue that industries should be concerned about is the flexibility of their process. Flexibility refers to the ability of the plant to operate over a range of conditions, while satisfying performance specifications (Swaney and Grossmann, 1985a). The more number of operating conditions the plant can operate at, the more flexible is the plant.

Resiliency is another feature of chemical processes that should be satisfied for the plants' optimal operation. Resiliency is the ability of the process to change smoothly from one operating condition to another. A resilient process should not suffer from major upsets and lead to losses that will affect the performance of the industry, while transitioning between operating conditions.

Grossmann and Morari (1983), through illustrative examples, show the significance of considering flexibility and resiliency at the design phase. They show that not always do commonly adopted design heuristics like over designing process equipment, adding new equipment, basing designs on worst operating conditions etc, which are supposed to improve the flexibility and resiliency of processes, lead to satisfactory performance. The design changes that occur as a result of this step might make the process infeasible and lead to losses for industry. So, they conclude that a systematic treatment of flexibility and resiliency is very important . Flexibility and resiliency analyses have not been conducted for the case studies examined, but suggestions to measure them have been made in Appendix E.

1.2 Feasibility and Operability Analysis

The main aim of this work is to evaluate process alternatives based on their feasibility and operability (F&O) and pick the best from the set of alternatives. F&O analysis is not limited to any one factor, but is a combination of multiple criteria like environmental impact, controllability, flexibility, resiliency and safety along with the profitability of the chemical process. The analysis helps in making a decision regarding the selection of the best feasible and operable design from a set of alternatives in industry. Now, the task is to find a tool that helps in selecting the best design based on multiple criteria.

Popular tools for multiple criteria decision making are Analytic Hierarchy Process (AHP) and Multi-Objective Optimization (MOO). These tools are discussed in detail in Appendix F. AHP supplies weights to the quantitative measures of each of the criteria and calculates an overall weighted average of operability. MOO finds an optimum solution by considering all objectives together and trying to find the best possible solution, which satisfies all objectives. Thus, both AHP and MOO require quantifying measures for all the criteria to perform the respective analyses and calculate the overall F&O index. This research aims at developing these quantifying measures to aid future work in adopting either AHP or MOO for an overall F&O analysis.

The unique contribution of this research comes in this phase of the work. Along with developing the quantifying measures for the F&O criteria, a simple approach is proposed for any process designed to be tested for its acceptability in industry. The approach to select a process design from a set of alternatives based on their profitability, environmental impact and controllability has been demonstrated with the help of two case studies as discussed in Section 1.1.

1.3 Collaboration with Industry

A major part of this work has involved input from industry. The motivating force behind the collaboration with industry is to adhere to the norm that research is done with the idea of advancing technology and implementing that work to benefit society. The principal mediators between research and society are industries, whose acceptance and implementation of the theoretical work determines the worth of any research. After the study and development of tools for the F&O criteria mentioned in the previous sections, an investigation was done on the current state of feasibility and operability analysis in industry. The responses from the industrialists allowed the expansion of the list of criteria for F&O, and gave a sharper focus to this research.

1.4 Motivation for This Research

The major motivation for this research is demonstrated in Figure 1.1. The worth of any chemical process with respect to the industrial scales depends to a large extent on its F&O characteristics.

In the previous work of this research group, an existing industrial process had been evaluated for its potential to cause environmental hazards. Using steady state simulation, the case was modeled and retrofit alternatives were generated. These alternatives were compared with the base case. One alternative was observed to be more environmentally safe and economical amongst all the alternatives. Hence, that alternative was chosen and recommended as a more appropriate processing strategy. This has satisfied just the feasibility criteria. However, the operability criteria need to be examined to determine if the alternative is worth implementing.

Very little work has been published where all the F&O criteria are considered together and used to compare alternative process designs. Operability alone has never

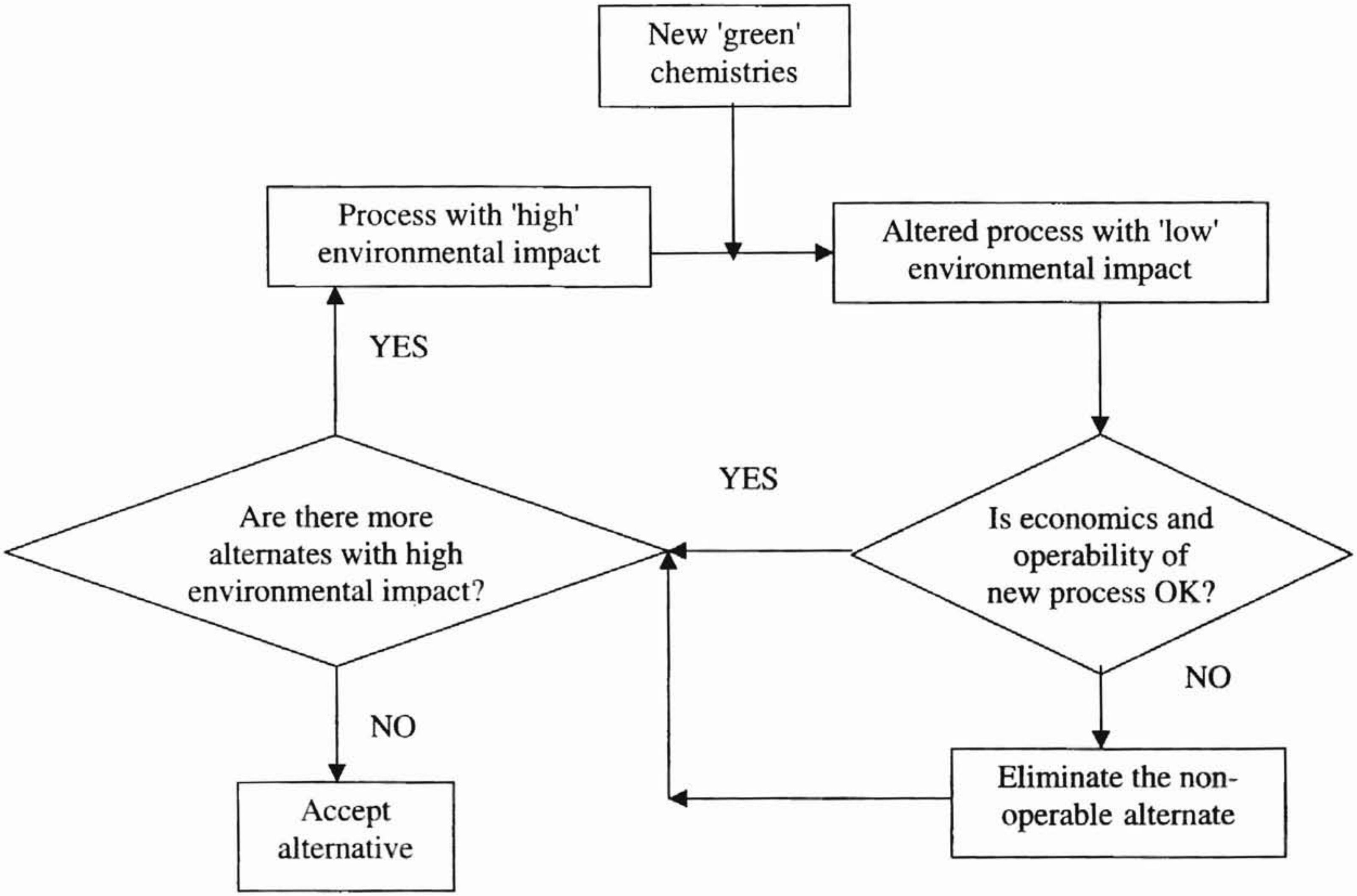


Figure 1. 1 Operability Analysis

been treated as a combination of not even all the criteria stated above[2]. This is proved by one of the latest reviews on operability by Schijndel and Pistikopoulos (1999). They listed 75 publications dealing with operability criteria and not one of them considered all the criteria together in comparing alternatives. Thus, the goal of this research is to develop a methodology to evaluate the F&O of any chemical process and compare the process with alternative designs. The motivation of any research is to generate results, which can be accepted and utilized in a productive manner by the society. The motivation of this research is no different from that. This research is aimed at carrying the evaluation of a process to its industrial feasibility to make it acceptable to industry and society in all respects.

The following chapters discuss the operability criteria more in detail. Chapter 2 gives a background of the research done to date in the area of operability. Chapter 3 presents some simple tools to evaluate controllability, environmental impact and profitability and these are illustrated with two case studies in Chapters 5 and 6. Chapter 4 discusses controllability measures. The industrial viewpoint is discussed in Chapter 7. The results of the research from the case studies and industrial input are given in Chapter 8. Based on the results in Chapter 8, some conclusions are drawn and recommendations made for future research in Chapter 9.

[2] A point to be aware of is that the list of operability criteria given above is not an exhaustive one, and there is always the scope of more criteria to be added depending on the specific requirements of the process, desires of the decision-maker (See Chapter 7). Thus the list should be flexible enough to be expanded.

Chapter 2

BACKGROUND

An industry is set up with intentions of manufacturing useful products and earning an income. Industries work hard to maximize profits. A lot of past work looked to enhance the profitability of the chemical processing industry. Many factors, which have an active role in the operation and economics of the industry, have been identified. Some of these factors are the ability to meet with the market requirements, the impact on environment, safety, flexibility, etc. The effects of these factors on the operability of the process have been studied individually and suggestions were made to nullify any negative effects. Several methodologies, which would enhance the operation of the industry, were developed to generate alternates to the existing processes. Based on the demanding requirements of the industry, the best alternate is chosen. For example, increasing profit might be the main objective of some processes while other processes need to be environmentally friendly.

This chapter gives a brief outline of the research done in the past in identifying the major influences on the feasible operation of industry in the face of any normal or abnormal conditions, or in other words on the feasibility and operability of chemical processes.

2.1 Feasibility Analysis

This section examines the work done in literature so far on feasibility of a chemical process in industry, where feasibility is coined to imply environmentally friendly and profitability. The process should have a low environmental impact to be acceptable to society and a high profitability to be acceptable to industry. Hence, these two aspects of feasibility are very crucial in deciding whether a process is worth implementing or not.

2.1.1 Environmental Impact

Protection of the environment is the primary concern of society and government. There has been a considerable amount of contribution in saving the environment from pollution. The government in its part has passed a number of laws and acts, which address various aspects of environmental pollution. Research in this area has been focussed on development of methods to minimize generation of waste in industrial processes. Douglas (1985) developed a new procedure for synthesizing process flow sheets and base-case designs. The procedure is evolutionary in nature and proceeds through a hierarchy of decision levels, where more fine structure is added to the flow sheet at each decision level. This was later extended to process synthesis for waste minimization (Douglas, 1992) which helps in the identification of potential pollution problems that the process may face in the initial stages of design itself.

Manousiouthakis and Allen (1995) also write that waste minimization is a process synthesis activity. This observation suggests that process synthesis concepts can help guide and accelerate the development of systematic waste minimization procedures, and waste minimization needs can help identify novel process synthesis problems. Ammann and coworkers (1995) suggest a frame work for environmental compliance both from engineering and economic perspectives.

The waste management hierarchy defined by EPA (Environmental Protection Agency) is source reduction, recycling, waste separation and concentration, energy and material recovery, waste treatment and waste disposal (Dantus, 1995). Traditionally end-of-pipe treatment has been favored for the reduction of environmental impact. The stress currently is towards removal of waste at the source itself. This will avoid the problem of disposing of waste in an environmentally safe manner after it is generated (end-of-pipe treatment). Companies are reluctant to apply source reduction techniques as they cost in terms of money, time and effort.

Dantus (1995; 1999) and van der Helm (1997) have addressed the problem of applying source reduction techniques for waste minimization. Industrial processes, which have a significant effect on the environment, and whose products and byproducts generated by these processes have been categorized as potential environmental hazards were selected for the study. Source reduction techniques were utilized to develop alternatives to replace existing industrial processes. Economic objectives were made a part of the overall methodology. thus ensuring that the new processes are certainly beneficial to the company. The general methodology to study the environmental impact of industrial processes that they adopted is development of a base case model, generation of process retrofit alternatives and economic evaluation of the alternatives.

Many other methods have been suggested to prevent pollution as a result of industrial processes. An integrated methodology is proposed for the design of industrial water systems (Alva-Argaez et al., 1998). This approach brings the engineering insights provided by the water pinch analysis together with powerful mathematical programming tools. Dyer and Mulholland (1998) suggest strategies that will improve reactor selectivity so that undesirable waste generating reactions are minimized while producing the desired product.

Mallick and coworkers (1996) listed three broad categories, of possible impacts on environment. These are: 1) environmental health impacts, 2) human health impacts and 3) resource depletion. They suggested a measure to calculate environmental impact as follows:

$$E_{i,l} = \sum_{x} \alpha_x \psi^s_{i,l,x} \qquad 2.1$$

where, $E_{i,l}$ is the relative potential environmental impact attributed to chemical, i, in stream, l, $\psi_{i,l,x}$ is the specific environmental impact of type x, α_x is the weighing factor placed on impact x and independent of the specific chemical. Then they developed a general theory for the flow and the generation of potential environmental impact through a chemical process (Cabezas et al., 1997). The theory defines six potential impact indices that characterize the generation of potential impact within a process, and the output of potential impact from a process.

Dantus (1999) modified this expression by ignoring α_x, and including a release potential factor, which is a function of the length of time for which the chemical is exposed to the environment. He calculated the environmental impact of the thermal chlorination of methane to give methyl chloride per kilogram of the product (methyl chloride) produced. In the current work, this expression is further modified by considering the release potential to be equal to 1.0 for all streams, and calculating the impact of each chemical in each stream of the process.

2.1.2 Profitability

Profitability of a chemical process is the main concern of industry. The operation of an industry highly depends on the ability of the process to generate a satisfactory income. The word, profitability is a general term for the measurement of the amount of profit that can be obtained from a given situation (Peters and Timmerhaus, 1991).

In comparing engineering investment alternatives, it is important to compare them over a common period of time (White et al., 1998). This period of time is called the planning horizon. The alternatives can be compared using a specified measure of worth. There are several methods of measuring investment worth. Some of them are (White, 1998):

1. Present worth method (PW): Converts all cash flows to a single sum equivalent at time zero. This is the most popular one as the reinvestment opportunities implied by present worth method or the net present value criterion are more realistic than any other method (Beaves, 1993). The conventional formula for present worth method presents a limited view of the concept, and hence, Beaves (1993) suggests a generalized or incremental formula for the present worth, which is less restrictive and overcomes issues such as mixed projects and reinvestment assumptions.
2. Annual worth method (AW): Converts all cash flows to an equivalent uniform annual series of cash flows over the planning horizon.
3. Future worth method (FW): Converts all cash flows to a single sum equivalent at the end of the planning horizon.
4. Internal rate of return method (IRR): Determines the interest rate that yields a future worth.
5. External rate of return method (ERR): Determines the interest rate that yields a future worth of zero.

6. Savings/investment ratio method (SIR): Determines the ratio of the present worth of savings to the present worth of investments.
7. Payback period method (PBP): Determines how long it will take to recover the initial investment.
8. Capitalized worth method (CW): Determines the single sum at time zero that is equivalent to a cash flow pattern that continues indefinitely.

Dantus (1999) compared 19 economic evaluation tools with 13 case studies. With this comparison, he showed that, the choice of a tool for economic analysis is not quite straight forward. The choice depends on the specific characteristics of the projects being evaluated and on the environment under which the decision is taken (certainty, risk, or uncertainty). In this comparison, he also shows that the annual worth method has one advantage over others. The advantage is that the annual worth method (also, known as annual equivalent profit, AEP) can be used regardless of the inequality of the projects' lives between the alternatives evaluated. For this reason, AEP is used as the economic analysis tool in this work.

In the 1980s as shareholders activism reached unprecedented levels, the concept of managerial compensation came into picture (Bacidore et al., 1997). The basic idea is that if managers are offered compensation contracts that are tied to shareholder wealth changes, their incentives will be better aligned with those of shareholders than is the case for other types of contracts. The choice of the financial performance measure in such a case would be the stock price, but stock price might not be an efficient one as it is driven by many factors beyond the control of the firm's executives (Milbourn, 1996).

Thus the financial performance measures used in managerial compensation should be highly correlated with changes in shareholder wealth, and the measure should not be subjected to all the randomness and "noise" inherent in a firm's stock price. For this the available performance measures are economic value added (EVA) and refined economic value added (REVA). EVA, proposed by Stern Stewart Management Services (Stewart, 1991), creatively links the firm's accounting data to its stock market performance. REVA is superior to EVA in that it assesses whether a firm's operating performance is adequate from the standpoint of compensating the firm's financiers for the risk to their capital (Bacidore et al., 1997).

The conventional economic analysis tools fall short when the impact of changing technologies needs to be evaluated. Strategic cost management method proposed by Shank (Shank, 1996) overcomes the limitations of conventional methods of capital investment analysis, which do not capture the full impact of the technology-change decision. A broader strategic cost management accounting approach was suggested by Shank by incorporating three additional tools into the capital budgeting approach: value chain analysis, cost driver analysis and competitive advantage analysis (Carr and Tomkins, 1996). Another approach to estimating costs related to changing technologies is activity-based costing (ABC), which breaks business functions into a series of discrete activities or processes, which correspond directly to elements in the cost of goods sold (Auguston, 1995). As a consequence, firms can get a more accurate estimate of the cash flows associated with a particular project. The key to a thorough economic evaluation is to develop an understanding of not only how the candidate systems perform economically, but also how each alternative fits into the overall enterprise and its strategic implications.

Since the stock performance of the firm or the effect of changing technologies need not be considered for this research, the above mentioned measures are not going to be employed. For the reasons stated earlier, annual equivalent profit is going to be used to conduct the economic analysis in this research.

2.2 Operability Analysis

Operability is the major area of interest for this research[1]. In simple words, operability of a plant can be defined as its ability to operate smoothly under any conditions. But this depends immensely on several factors like controllability, flexibility, resiliency and safety of the process. The main aim of this section is to show that operability analysis has always been done by considering only individual, or a few criteria, and not all of them together. Operability analysis based on individual criteria or few criteria gives an incomplete study of the feasibility of the process in industry as no process can be declared perfectly operable if for example, it is just tested for flexibility and safety and not for others.

The following section exclusively deals with controllability as it is one of the major interests of this research.

---

[1]Operability of a chemical process are vast areas of studies and it is beyond the scope of this research to study all aspects. Hence, only the controllability aspects of operability have been dealt with in this work. Quantitative measures have been suggested for flexibility, resiliency and safety in Appendix E. Application of these quantifying measures and the development of an overall operability index have been recommended for future work.

2.2.1 Controllability

Extensive work on controllability has been presented in literature. The main aim was to provide good control to industrial processes and enhance their performance efficiency in the face of any kind of disturbances or upsets. Work has been done to evaluate the controllability of designs, test the efficiency of the control strategies used to control the process and also to compare alternate designs and strategies to help pick the best.

2.2.2 Design and Control

Stress has always been laid on designing control systems along with the design of the process as that would help avoid faulty process designs causing control failure (Shinskey, 1983). Fisher and coworkers (1988a; 1988b; 1988c) in a series of papers showed that controllability analysis should be performed at the preliminary stages of process design so that the economic penalties associated with control could be used to screen process alternatives. Huang and Fan (1992) propose a distributed strategy to actively integrate the design of a process network and its control. Belanger and Luyben (1998a; 1998b; 1998c) in a series of three papers explore the design and control of processes containing inert components.

Tyreus and Luyben (1999) suggest three approaches to integrate process design and control: hierarchical approach, thermodynamic approach and optimization approach. With the three approaches, they show how design decisions can affect the dynamic operability of the resulting process design.

2.2.3 Controllability Measures

In order to compare alternate designs based on their controllability, there is a need for a measure to evaluate controllability. Some popular controllability measures found in literature are:

- Relative gain array developed by Bristol (1966) who was the pioneer in developing a quantitative measure to evaluate the controllability of a design. The array gives an approximate measure of the design's sensitivity to disturbances and helps in picking a good control structure too.
- Perkins and Wong (1985) used the theory of functional controllability as a measure of the effect of time delays on control performance. Time delays in a process hamper the achievement of good control. For single input single output systems, the longer the delay the worse the degradation in control performance. The idea underlying the theory of functional controllability is to investigate conditions under which a desired trajectory for the outputs from a plant may be specified, and inputs found which generate the desired trajectory (Perkins and Wong, 1985).
- In contrast to single variable systems, for multivariable systems increasing delays in elements of a transfer function matrix results in better control performance (Grossmann and Morari, 1983).
- Shimizu and Matsubara (1985) utilized a new measure for controllability, which requires developing a gain matrix in place of a relative gain array and performing singular value analysis (SVA) on the matrix. SVA helps in finding a good control structure for the system. In their paper, four control structures for the conventional

distillation column were assessed, and the effect of directions of disturbances and modeling errors on control quality was studied.

Singular value analysis has since then been extensively used to not only find a good control strategy (i.e., a good combination of controlled and manipulated variables) for one particular process design (Seborg et al., 1989), but also for designing simple but effective multi variable control systems (Moore, 1986), and to evaluate the controllability of alternative process designs based on the process condition number (Barton et al., 1986).

- Weitz and Lewin (1996) developed a short cut diagnostic tool to assess the controllability and resiliency of a process flowsheet. The approach involves deriving a linear dynamic model of the process from steady state information.

2.2.4 Steady State Versus Dynamic Evaluations of Controllability

Another important issue that needs to be considered is whether evaluation of designs for controllability should be done at steady state or dynamic operating conditions. A lot of work has been done in both areas. Fisher and coworkers (1985b) made major contributions in this field. They evaluated significant economic trade-offs for process design and steady state control optimization problems. They also presented a preliminary steady state control structure synthesis procedure (Fisher et al., 1984) and demonstrate the advantages of initiating control studies with a steady-state analysis (Fisher et al., 1985b). Morari (1983a) gave a general framework for controllability assessment based on a linear analysis of the fundamental limitations to control performance.

Narraway and coworkers (1991) were the first to study the interaction of process design and control in the light of the effect of the interaction on economics under dynamic conditions. Also, they presented a method to select process control structure based on linear dynamic economics (Narraway and Perkins, 1993). From this review, it could be concluded that though, when ill-behaved dynamics or constraints are the primary control-related problems, dynamic models for control offer distinct advantages, steady state models can deliver similar advantages with considerably less effort when nonlinear or nonstationary effects are the primary control problems (Ramchandran, 1998).

2.2.5 Operability Studies

This section presents the work that has been done in literature on operability. As mentioned in Chapter 1 (See Section 1.1), operability definition has varied from author to author in that each defines operability based on a different set of criteria. The following discussions show the different ways in which operability has been defined.

Lennhoff and Morari (1982) proposed a new design approach to improve the economic efficiency of plant operation. The approach stresses on the consideration of steady state economic and operational/dynamic aspects simultaneously, rather than individually. They aimed at designing alternatives and choosing that design and control structure which is best operable. They also formulated a resilience index, which is a measure of the largest disturbance that the network can tolerate without becoming infeasible (Saboo and Morari, 1984b).

Morari (1983b) reviews techniques, which attempt to exclude the engineer and automate the design process, to develop more flexible processes. Flexibility, operability and controllability should be included in the design stage itself, as it is very difficult to operate plants at nominal design conditions or steady state. Grossmann and coworkers

(1983b) discuss the optimization strategies required for designing flexible chemical processes. They considered flexibility, controllability, reliability and safety of the chemical plant to be the important operability criteria that need to be studied at the design stages to ensure that the plant still meets with the economic specifications. This work by Grossmann and coworkers is the one of the first work in literature that identifies more than three criteria for operability, though they studied flexibility alone, extensively.

Grossmann and Morari (1983a) define operability as the ability of the plant to perform under conditions different from the nominal design conditions. In their work they mainly dealt with flexibility (feasibility of steady state operation for a range of different feed conditions and plant parameter variations) and resiliency (safe and reliable operation despite equipment failures) of the plant. They concluded from their work that the traditional approach of over designing equipment to improve the plants' flexibility and resiliency may sometimes work to the contrary and also, might prove to be expensive. Design changes can have very pronounced, but difficult to predict effects on the sensitivity of the performance of a controlled system to modeling errors and thus on the dynamic resilience.

Harris (1993) discusses quality issues in process design and operations. He writes that quality can be improved by reducing product variability, along with focussing on the customer needs and expectations. He shows that there is a common framework to analyze many process monitoring methods.

Morari and Perkins (1995) gave an excellent review of effects of design on controllability from mid 80s to mid 90s. They reviewed the different approaches that have been used and identified some future needs. One major future need is that there is an immense need to develop simple criteria for controllability evaluation, which will help in formulation of a meaningful algorithmic synthesis technique to trade off controllability and economics. They advise against the removal of the engineer from the loop to develop 'automatic synthesis' as suggested by Morari himself (Morari, 1983).

Schijndel (1999) in an extensive review of the literature on operability discussed the work that has been done so far on operability criteria, interaction of design and control, plant wide control, control structure selection and availability and maintenance. From the observations that he made he concluded that there is an urgent need to bridge the gap between academic theory and industrial practice in the field of process design and operability. This bridging requires a coordinated effort between industry and academia in properly defining the needs and demonstrating the benefits to key business/industrial applications. This research has conducted an industrial survey too (See Chapter 7).

2.2.6 Operability Measures

This section discusses the quantifying measures for operability available in literature.

- Swaney and Grossmann (1985a) developed a measure for flexibility, which they considered one of the key components for operability. They presented a general framework for analyzing flexibility in chemical process design, and formulate a flexibility index which, is a measure of the size of the region where feasible steady state operations can be performed (See Figure 2. 1).

  The region, $\psi(d,\theta) = 0$, is the feasible operating region and θ are the uncertain parameters (which are the disturbances, and changes in input variables). The changes in θ are considered to be the same in both positive and negative

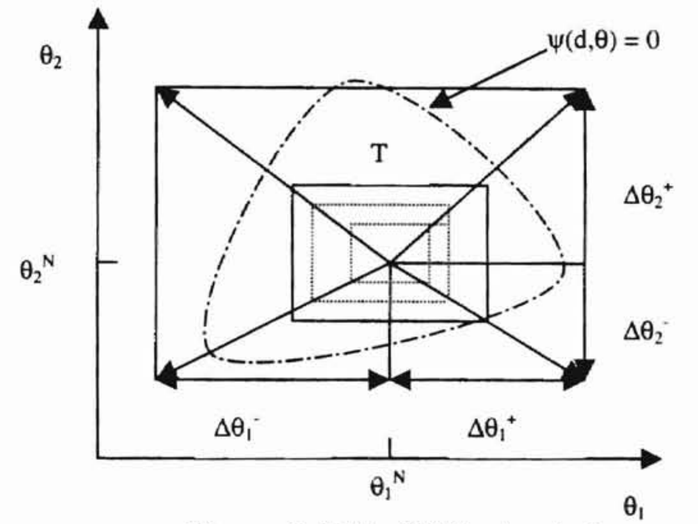


Figure 2. 1 Flexibility Analysis

directions and are represented by a single variable, δ. As δ increases, a series of rectangles are inscribed within the feasible region as shown in Figure 2.1. The flexibility index is the value of δ that produces the maximum inscribed rectangle in terms of area.

This quantification measure for flexibility and an extension to it are discussed in detail in Appendix E. They also gave procedures for the numerical computation of the flexibility index (Swaney and Grossmann, 1985b). The algorithms that they developed were also proved to be sufficient with several examples.

- Terrill and Douglas (1987) consider process operability studies at steady state conditions as an effective way to pick the best alternative for a heat exchanger network.
- A hazard and operability study, or HAZOP, reviews both the design and operation of a facility, identifying potential hazards and/or problems with plant operability (Goyal,

1993). Goyal in his article on HAZOP gives a list of techniques and planning rules to perform a HAZOP study for a process. Some computer software packages utilized for the purpose are HAZOP-PC and HAZSEC-PLUS. HAZOP is one of the hazard identification techniques under OSHA (Occupational Safety and Health Administration).

- Rovaglio and coworkers (Rovaglio et al., 1995) identify controllability, observability and flexibility as relevant operational indices and demonstrate their studies by using an azeotropic heterogeneous system. They define stationary and dynamic operability indexes as an extension of the work done by Swaney and Grossmann (1985a; 1985b).
- Downs and Ogunnaike (1995) in an interesting paper on the interaction between design, control and operability write about product quality being measured as product variability as one of the most important criterion for operability. The ability of plants to exhibit stable, low variability operation will become a major factor in discriminating between competing designs.
- Chacon-Mondragon and Himmelblau (1996) describe the importance of shifting focus from cost savings alone to cost savings and flexibility, while maintaining the controllability of the process, as criteria for operability during design of a process. They developed a flexibility index called Lebesque measure, which is a measure of the region available for operation within the process constraints (See Figure 2.2). Figure 2.2 shows a system where the total cost is being minimized and the flexibility index is being maximized.

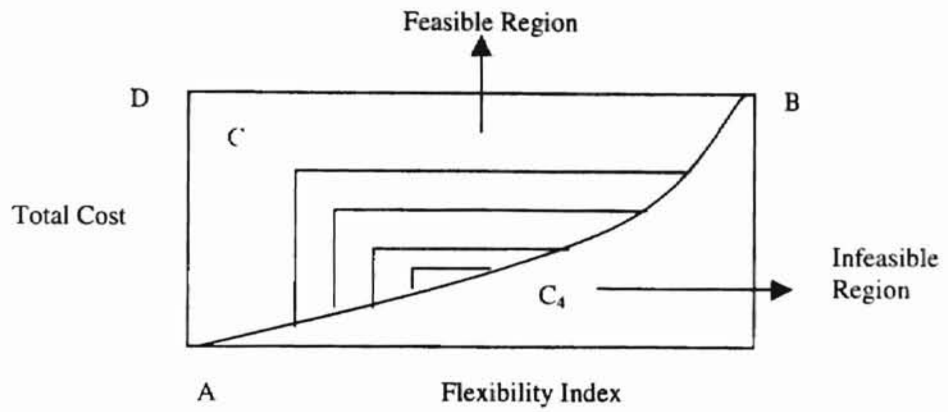


Figure 2. 2 Cost Savings and Flexibility

The region AC_4BD represents all the feasible operating points within the objective function space. The measure of the region, AC_4BD, is the Lebesque measure.

- Operability of a process can be improved and money can also be saved by integrating design and control, rather than adding control on top of a finished design (Pumps, 1996). An integrated methodology is presented to consider different issues of operability assessment, especially flexibility and controllability by Bahri and coworkers. (1997). They proposed a framework within an optimization environment, which incorporates optimality along with controllability and flexibility.
- Ostrovsky and coworkers (1996) modified the flexibility function of chemical processes that Grossmann proposed, to give a simpler and more effective method to calculate the flexibility.

2.3 Summary

This chapter gave a background of the work done in environmental impact, controllability and operability studies of chemical processes. Section 2.1 presented the work that has been done till now on feasibility studies, which is coined for the environmental impact (Section 2.1.1) and profitability (Section 2.1.2) studies in this research. Work on suggestions to reduce the hazards due to environmental impact and also measures to quantify the impact on environment are given.

Section 2.2 discusses the work done on operability till date. Section 2.2.1 was devoted to controllability. The popular concept of interaction between process design and process control, and a comparison between steady state and dynamic evaluations are discussed. The controllability measures that have been studied so far in literature are also discussed.

The second part of Section 2.2 discusses the work done in operability and the various measures that were studied to measure operability. This section explains the work done so far and how it is going to be followed up in the current research.

Chapter 3

FEASIBILITY AND OPERABILITY

This Chapter discusses the major contributions of this work. The feasibility and operability criteria that have been gathered are discussed briefly. Quantitative measures used to evaluate environmental impact and profitability (feasibility criteria) and controllability (one of the criteria for operability) are discussed in detail. Finally an example problem was used to demonstrate the quantification measures developed for the three criteria.

3.1 Introduction

This chapter gives an outline of the major contributions of this research work. The following section discusses the objectives of this research.

3.1.1 Objectives of this research

The objectives of this research have already been discussed in Section 1.1. The objectives relevant to this Chapter are:

- Formulate a comprehensive list of criteria that an industrial process should satisfy to be able to operate smoothly under any conditions and to evaluate alternatives.
- Conduct a qualitative and quantitative study of the feasibility criteria and controllability, and develop measures to quantify them.

- Treat those criteria that cannot be quantified subjectively and utilize them to compare alternative designs when the process of elimination brings the available choices of designs to a small number.
- Compare alternative process designs and select the design that is the best in terms of environmental impact, profitability and controllability for which the alternatives are being evaluated.

In other words, the focus of this work is to develop a systematic procedure to conduct **feasibility and operability** (F&O) analysis of a chemical process. As discussed in the previous chapters, feasibility is coined in this research to imply the acceptability of the process to industry as far as its profitability is concerned and to society with respect to the process's impact on the environment. Operability of an industrial process, in simple words, measures the ability of a chemical process to function smoothly in industry. The general term, operability, is used to describe the ability of the plant to perform satisfactorily under conditions different from the nominal design conditions (Grossmann and Morari, 1983).

Following section gives the feasibility and criteria gathered initially in this research.

3.1.2 Initial Feasibility and Operability Criteria

Based on an extensive literature survey and personal insight, a list of F&O criteria has been put together at the beginning of this research. These criteria are given below.

The feasibility criteria are:

- Profitability ($)
- Environmental Impact (E)

The operability criteria gathered are:

- Controllability (C)
- Resiliency (R)
- Flexibility (F)
- Safety (S)

The above list of F&O criteria is certainly not an exhaustive one. For such intricate processes as the industrial chemical processes, there will certainly be many more factors that need to be studied. For this reason, a questionnaire has been sent out to 75 industries, the main query being with what criteria do they evaluate process designs when they perform operability studies in their industries. The results and conclusions of this survey are given in Chapter 7. The unique contribution of this work is that it tries to encompass all the essential factors that any chemical process should be evaluated upon, instead of individual criteria as is found in literature (See Chapter 2).

Profitability, environmental impact and controllability are most influential in decision making when selecting the best design from a set of alternatives because: 1) Industries are most interested in the profitability of a process. 2) The concept of reducing environmental impact is becoming very popular and more and more stringent environmental laws are being enforced. 3) If the plant is not controllable, the plant may have to be shut down completely. For these reasons, this work mainly focuses on these three criteria ($, E and C).

Systematic procedures were developed to evaluate chemical processes based on these three criteria in the following sections and demonstrated with an example problem in Section 3.5. These have been coded in ASPEN PLUS™. The ASPEN PLUS™ code was made as general as possible. So, a run in ASPEN PLUS™ following the steps in the methodology section (See Appendix A) will give the values of the controllability and environmental indices along with the profit generated. The developed methodology has been tested with two cases, a hot and cold water mixing system (See Chapter 5), and manufacture of methyl chloride (See Chapter 6). The following sections give the detailed descriptions of \$, E and C.

3.2 Controllability Analysis

Controllability is defined as the ability of the plant to easily reject any disturbances upsetting the system and meet with the set points. Controllability analysis is very crucial for the smooth operation of industry. As shown by Shinskey (1983), processes can become uncontrollable due to several reasons like negative resistance (lack of steady state stability), exothermic reactions, lack of uniform coolant velocity in the jackets of stirred tank reactors and interaction between parallel unit operations.

There are several ways to evaluate the controllability of a process, but the tool chosen for this work was **Singular Value Analysis (SVA)**. Before discussing SVA, some definitions need to be discussed.

3.2.1 Definitions for Control Studies

Controlled Variables (*CV*): These are the output variables that need to be maintained at desired set points.

Manipulated Variables (*MV*): These are the variables which are changed in order to bring the controlled variables to their set points.

Disturbance Variables (*DV*): These variables upset the system and tend to deviate the CV from their set points.

Degrees of Freedom (*DOF*): Degrees of freedom is the difference in total number of process variables (unspecified inputs plus outputs), and the number of independent equations (Seborg et al., 1989).

3.2.2 Singular Value Analysis

Singular value analysis helps in picking a good control strategy (combinations of controlled and manipulated variables) as well as in choosing the best design in terms of controllability from a set of alternatives[1]. A control strategy is designed by choosing appropriate combinations of CV and MV, i.e., those combinations in which MV has a good influence on the CV. A measure of controllability called **Condition Number (*CN*)** is used to determine the "goodness" of the combination of CVs and MVs. Singular value analysis is performed to determine the condition number of each design. Some of the conditions that SVA tests for are:

- Number of manipulated variables (MV) should be more than or equal to the number of controlled variables (CV).
- Manipulated variables should have a stronger influence on controlled variables than disturbance variables (DV).
- Controlled variables should be sensitive to changes in the chosen manipulated variables.

The mathematical development of SVA is given below.

A linearized steady state model can be expressed as follows (Seborg et al., 1989):

$$\Delta CV = K \Delta MV \qquad 3.1$$

where, ΔCV is the vector of deviations in n controlled variables, ΔMV is the vector of deviations in n manipulated variables, and $\boldsymbol{K}$ is the steady-state gain matrix.

Steady state gain is defined as the ratio of the deviation of output variable to that of the input variable; or the ratio of the deviation of the controlled variable to that of the manipulated variable; or

$$K_{ij} = \frac{\Delta CV_i}{\Delta MV_j} \qquad 3.2$$

In order to make the elements of the matrix dimensionless, the deviations are normalized in the following manner:

$$K_{ij} = \frac{\Delta CV_i / CV_i}{\Delta MV_j / MV_j} \qquad 3.3$$

The steady state gain matrix is the matrix containing ixj elements, K_{ij}, each representing the effect of deviation of a manipulated variable, MV_j on a controlled variable, CV_i.

The steady state gain matrix for any system is developed as shown below.

The control strategies are designed by pairing MV and CV as follows:

$MV_1 \Rightarrow CV_1$ i.e., MV_1 controls CV_1

$MV_2 \Rightarrow CV_2$, i.e., MV_2 controls CV_2 and so on.

The general matrix formed by MV and CV appears as shown in Table 3.1.

---

[1] SVA can be treated as a simple preliminary tool for controllability analysis. See Chapter 4 for more

Table 3. 1 General Steady State Gain Matrix

	MV_1	MV_2	$...MV_r$	$...MV_n$
CV_1	K_{11}	K_{12}	$...K_{1r}$	$...K_{1n}$
CV_2	K_{21}	K_{22}	$...K_{2r}$	$...K_{2n}$
$...CV_r$	K_{r1}	K_{r2}	$...K_{rr}$	$...K_{rn}$
$...CV_n$	K_{n1}	K_{n2}	$...K_{nr}$	$...K_{nn}$

In Table 3.1, each element of the gain matrix can be represented as Equation 3.3, or

$$K_{ij} = \frac{(CV_i - CV_{iO}) / CV_D}{(MV_j - MV_{jO}) / MV_D} \qquad 3.4$$

where D = maximum acceptable deviation of the variable from optimum values which the variable can maximum change, and

O = initial steady state optimum value of the variable

As a rule of thumb, all equipment are designed in a way so as to accommodate 20% plus or minus the required amounts. So, the ranges that are chosen for this system are also 20% plus or minus of the optimum values.

An important property of the matrix $\boldsymbol{K}$ is its singular values, $\sigma_1, \sigma_2, \ldots \sigma_n$. The singular values are defined as the positive square roots of the eigenvalues of $K^T K$. They are a measure of how close the matrix is to being singular, i.e., to having a determinant of zero (Luyben and Luyben, 1997). Usually, the nonzero singular values are ordered with σ_1 denoting the largest and σ_r, denoting the smallest.

The condition number is defined as the ratio of the largest and the smallest nonzero singular values:

details.

$$CN = \sigma_1 / \sigma_r \qquad 3.5$$

A process is said to be ill conditioned if $\boldsymbol{K}$ is singular and by convention, $CN=\infty$ for such a process.

The condition number is a positive number that provides a measure of:

- how ill conditioned the gain matrix is
- sensitivity of the matrix properties to variations in the elements of the matrices. The CV should be sensitive to changes in MV as otherwise, an infeasible and uneconomically large change might have to be made in MV to control the CV. Thus, an ill-conditioned matrix implies that the corresponding process is not controllable, or the control strategy chosen to control the process is not a suitable one.
- A high condition number means that irrespective of the control strategy chosen its impractical to satisfy the entire set of control objectives.

Thus, SVA helps in calculating *CN* for each alternative strategy/design and depending on which has a lower value of *CN*, the better one can be proposed.

3.3 Environmental Impact

Environmental impact criterion assesses the impact of the chemical process on the surrounding environment. In the light of the increasing demand for benign chemical processes from the government and other organizations, there is a growing need to make the processes less hazardous to the environment. The impact of the process on the surrounding environment is calculated by estimating the impact of each chemical present in each stream of the process. The expression used to calculate the impact is (Dantus, 1999):

$$E = \frac{\sum_{i=1}^{n}\sum_{j=1}^{m} r_i w_i m_{j,i} \phi_j}{P} \tag{3.6}$$

where,

E = Environmental Impact (EIU/kg)

EIU = Environmental Impact Units

r_i = release factor

w_i = flow rate of waste stream i (kg/hr)

$m_{j,i}$ = mass fraction of component j in waste stream i

ϕ_j = environmental impact index of chemical j (EIU/kg) (a function of effects on human health, environment and exposure potential)

P = total mass of product obtained (kg/hr)

The release factor (r_i) accounts for the release potential of the waste stream, i. The factor's value varies between 0 and 1 depending on the particular stream. For waste streams, $r = 1$, whereas for non-waste streams, $0 \leq r \leq 1$. The environmental impact index (ϕ_j) is a measure of the effect of the process on human health, environment and the length of time it is exposed to the environment. Davis and coworkers (1994) calculated the environmental impact index with the expression:

$$\phi = (\text{Human Health Effect} + \text{Environmental Effect}) \times (\text{Exposure Potential}) \tag{3.7}$$

where,

$$\text{Human Health Effect} = HV_{\text{oralD50}} + HV_{\text{inhalation LC50}} + HV_{\text{carcinogenity}} + HV_{\text{other}} \tag{3.8}$$

$$\text{Environmental Effects} = HV_{\text{oralD50}} + HV_{\text{fish LC50}} + HV_{\text{fish NOEL}} \tag{3.9}$$

$$\text{Exposure Potential} = HV_{BOD} + HV_{hydrolysis} + HV_{BCF} \quad 3.10$$

where, HV stands for Hazard Value. Definitions of the hazard value (HV) terms in the above equation can be obtained from the work of Dantus (1999).

Davis and coworkers have compiled the data for about 161 chemicals for calculation of the environmental impact index in the Toxics Release Inventory. As of 1995, data for 656 chemicals are reported under the Toxics Release Inventory (Dantus, 1999). Data to calculate the environmental impact index are taken from the works of Davis (1994) and for $HV_{carcinogenity}$ and HV_{other} in specific, Bouwes (1997a; 1997b).

3.4 Profitability

Profitability is generally the principal deciding factor of the acceptance or rejection of a process design. There are many tools available to measure the profitability of any process. The tool chosen for this work was Annual Equivalent Profit (*AEP*). Dantus (1999) compared 19 economic tools with 13 case studies and showed that choosing an economic tool is not very straight forward as the choice depends on specific characteristics of the project. Among all the tools, one apparent advantage that AEP has over other economic tools in comparing alternatives is that this tool can be used regardless of the inequality of the projects' lives. Hence, *AEP* was chosen for this research.

Also, known as the annual worth method, *AEP* converts all cash flows to an equivalent uniform annual series of money for a certain period of time (Canada et al., 1996). *AEP* is calculated by the expression

$$AEP = NPV * A_f \quad 3.11$$

where, NPV = Net Present Value

A_f = Annual Worth factor

The determination of the net present value involves the summation of each individual cash flow converted to its present worth equivalent to obtain the net present value. NPV is calculated by the expression

$$NPV = \sum_{n=0}^{N_y} \frac{CF_n}{(1+i_r)^n} \quad 3.12$$

where, CF = cash flow

i_r = interest rate

n = number of current year

For year $n = 0$, cash flow considers the fixed (F_c) and working capital (W_c), where the fixed capital is the cost of equipment and, working capital is the inventory costs (Stermole, 1996).

For $n = 1$ to N_y, positive cash flow or cash inflow (CF_i) is from the revenue obtained from selling the product (CH_3Cl). Negative cash flow or cash outflow is due to the following costs (Dantus, 1999):

1. Raw material costs: Cost of CH_3OH + HCl
2. Utilities costs: Feed preheating costs + Cooling water costs
3. Waste related costs: Cost involved in treating and disposing of waste.

Depreciation (F_d) is calculated by the straight line method given by:

$$F_d = \frac{F_c - F_s}{N_y} \quad 3.13$$

where, F_s = salvage value

Though depreciation is a positive cash flow, it should be added as a cost when calculating the taxable income. Taxable income *(TI)* is the difference in the cash inflow and the cash outflow and the depreciation (Stermole, 1996):

$$TI = CF_i - CF_o - F_d \qquad 3.14$$

Net income *(NI)* is the income left after the tax charges are deducted from the taxable income:

$$NI = TI * (1 - T_x) \qquad 3.15$$

where, T_x = tax rate.

Finally, cash flow is the net income plus the depreciation charges:

$$CF = NI + F_d \qquad 3.16$$

This is then substituted in Equation 3.12 to calculate NPV.

Annual worth factor is given by the expression:

$$A_f = \frac{i_r(1+i_r)^{N_y}}{(1+i_r)^{N_y} - 1} \qquad 3.17$$

where, N_y = project life time. *NPV* and A_f are then substituted in Equation 3.11 to calculate AEP for each alternative.

The annual equivalent profit thus calculated using the above equations is used to compare alternate designs and select the most profitable one.

3.4.1 Assumption Made in the Above Analysis

The main advantage of using Annual Equivalent Profit is that the tool allows for the comparison of alternate designs regardless of the length of their lives, unlike other economic tools like Net Present Value (NPV), which requires that all designs have the same length of life. The assumption made in using this tool is that the length of life of each design is the least common multiple of the lives of all the alternatives (White et al., 1998).

The previous sections gave detailed quantitative analyses for the three criteria: controllability, environmental impact and profitability. The quantitative analyses are illustrated with an example in the next section. A critique of the controllability measures adopted in this work and the available ones in literature is given in the following chapter. The code developed for the analysis has been tested on two case studies, which are discussed in Chapters 5 and 6. Quantitative measures were suggested for flexibility, resiliency and safety in Appendix E.

3.5 Example Calculations of Controllability, Environmental Impact and Profitability

This section demonstrates the utility of the tools developed in the previous sections for controllability, environmental impact and profitability analyses.

3.5.1 System

The example calculations are conducted for the reaction given by Equation 3.16.

$$A \rightarrow B + C \qquad 3.18$$

In this system, A is the reactant, B is the main product and C is the by-product. Figure 3.1 gives the flowsheet of the process.

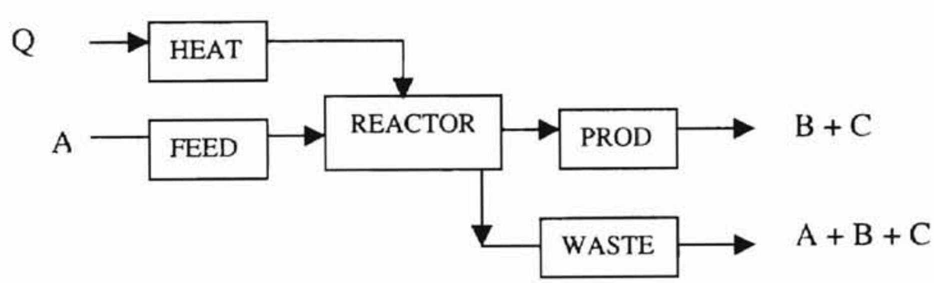


Figure 3. 1 Flowsheet of Example System

The FEED stream consists of pure A and is fed to a reactor. The HEAT stream supplies heat to the reactor and helps in the maintenance of the temperature of the reactor.

The effluent streams from the reactor are PROD, which contains B & C and the WASTE stream, which contains unreacted A and, B and C that could not be retrieved in the PROD stream. The aim is to produce B at a rate of 55kg/s and maintain the temperature of reaction at 1000K at a pressure of 5atm.

The system input values are as follows:

FEED flowrate = 80kg/s

HEAT supply = 1200J/gmol

3.5.2 Singular Value Analysis

The desired product (B) flow rate is 55kg/s and the temperature should be maintained at 1000K. Hence, the controlled variables are:

$$CV1 = PROD$$

$$CV2 = TEMP$$

where, *PROD* = flowrate of B, kg/s

TEMP = temperature of reaction, K

The flowrate of A was chosen as the manipulated variable to control the flowrate of B, and the heat supply to the reactor as the manipulated variable to control the temperature of the reaction. Hence, the manipulated variables are:

$$MV1 = FEED$$

$$MV2 = HEAT$$

The acceptable deviations of the *CV*s and *MV*s were considered to be 20% of the initial steady state optimum values. The operating ranges and acceptable deviations of the CVs and MVs are shown in Table 3.2.

Table 3. 2 Acceptable Deviations and Operating Ranges of CV and MV

	Initial Steady State Optimum Values (XV_O)	Acceptable Operating Ranges (XV_R)	Acceptable Deviations from Initial Optimum Values (XV_D)
CV_1 (kg/s)	50	40-60	10
CV_2 (K)	1000	800-1200	200
MV_1 (kg/s)	80	64-96	16
MV_2 (J/gmol)	1200	960-1440	240

where, *XV* stands for *CV* or *MV*.

In order to observe the effect of the *MV*s on *CV*s, the values of each of the manipulated variables are increased by 10%, individually. This action automatically deviates the controlled variables from their optimum values. Table 3.3 gives the results of increasing MV1 and MV2 respectively by 10% from their initial steady state optimum values.

The results in the third column in Table 3.3 are obtained by increasing MV_1 by 10% of its initial steady state value while keeping MV_2 at its initial value. Similarly, the results in the fourth column in Table 3.3 are obtained by increasing MV_2 by 10% of its initial value and keeping MV_1 at its initial value.

Table 3. 3 Effect of Increasing MV_r by 10% of its Initial Steady State Optimum Value on the CVs

	Initial Steady State Optimum Values (XV_O) ($XV = XV_O$)	New Values after *MV1* is Changed (XV_i) ($MV2 = MV2_O$)	New Values after *MV2* is Changed (XV_i) ($MV1 = MV1_O$)
CV_1 (kg/s)	50	60	52
CV_2 (K)	1000	1025	1100
MV_1 (kg/s)	80	80.8	80
MV_2 (J/gmol)	1200	1200	1212

Using Equation 3.4,

$$K_{ij} = \frac{(CV_i - CV_{iO})/CV_D}{(MV_j - MV_{jO})/MV_D} \qquad 3.4$$

the steady state gain matrix elements, K_{ij}, are calculated. K_{ij} is the steady state gain value obtained as a result of the effect of MV_j on CV_i.

For example, $K_{12} = \dfrac{(CV_1 - CV_{1O})/CV_D}{(MV_2 - MV_{2O})/MV_D} = \dfrac{(52-50)/10}{(1212-1200)/200} = 3.33$

In a similar manner, other elements of the gain matrix are also calculated and the resulting matrix is given in Table 3.4.

Table 3. 4 Steady State Gain Matrix, *K*, for the Example System

	MV1 (FEED)	*MV2 (HEAT)*
CV1 (PROD)	20	3.33
CV2 (TEMP)	2.5	10

This matrix is now subjected to singular value analysis (by any standard SVA algorithm (Press et al., 1992), or by using packages like Mathcad). The resulting singular values are: $\sigma_l = 20.793$ and $\sigma_r = 9.218$

The condition number is calculated using Equation 3.5,

$$CN = \sigma_1 / \sigma_r \tag{3.5}$$

$$CN = 20.793/9.218 = 2.26$$

This value of CN (2.26) represents the amount of conditioning of the gain matrix or in other words, the number is a measure of the influence of MV on CV. The higher the value of CN, the lower is the influence of MV on CV. When a new control strategy is designed and the CN for that strategy is calculated, the strategies can be compared. The strategy having the lower CN is the better one.

Following section gives sample calculations of environmental impact.

3.5.3 Environmental Impact

Environmental impact of the example system is calculated by Equation 3.6,

$$E = \frac{\sum_{i=1}^{n} \sum_{j=1}^{m} r_i w_i m_{j,i} \phi_j}{P} \tag{3. 6}$$

The environmental impact index values (ϕ_j) for all the chemicals in the system are given in Table 3.5.

The mass flowrates (w_i) of stream i and mass fractions (m_{ji}) of component j in stream i are given in Table 3.6.

Using Equation 3.6, the impact of the example system on the environment is calculated. The release factor is assumed to be 1.0 for all streams.

Table 3. 5 Environmental Impact Index Values for the Example System

Chemical in the Example System	Environmental Impact Index (EIU/kg) (ϕ_j)
A	25
B	40
C	10

Thus,

$$E = \frac{\sum_{i=1}^{n}\sum_{j=1}^{m} r_i w_i m_{j,i} \phi_j}{P} = \frac{[80\times1.0\times(1.0\times25+0.0\times40+0.0\times10)]+[55\times1.0\times(0.0\times25+1.0\times40+0.0\times10)]+[25\times1.0\times(0.29\times25+0.06\times40+0.65\times10)]}{55}$$

$= 83.7$ EIU/kg

The value of E (83.7 EIU/kg) represents the amount of impact that this system has on the environment for every kg of product produced. When an alternate is designed and the E for that design is calculated, the design that is more friendly to the environment is determined by the one that has a lower value of E.

3.5.4 Profitability

Profitability of the example system is calculated by Equations 3.11 to 3.17 for a project life (N_y) of 5yrs. The major component of the profitability calculation is the calculation of the cash flow, CF.

The data required to calculate the cash flow is (CF) given below:

Tax rate (T_x) = 0.35

Interest rate (i_r) = 0.1

Table 3. 6 Mass Flowrates of Streams (w_i) and Mass Fractions (m_{ji}) of Components in the Streams of the Example System

	FEED (Stream 1)	PROD (Stream 2)	WASTE (Stream 3)
Stream Flowrate (w_i, kg/s)	80	55	25
Mass fraction of A in stream, i ($m_{A,i}$)	1.0	0.0	0.29
Mass fraction of B in stream, i ($m_{B,i}$)	0.0	1.0	0.06
Mass fraction of C in stream, i ($m_{C,i}$)	0.0	0.0	0.65

For year $n = 0$, the cash flow is the fixed capital alone. Thus,

$CF_0 = F_c = 10000\$ = 1E\text{-}2$ M\$/yr

The costs of all the chemicals in the system are given in Table 3.7.

Table 3. 7 Economic Data for the Example System

	Chemicals	Cost (\$/kg)
Chemical costs	A	0.5
	B	1.1
	C	0.4
Waste related costs	Waste Treatment Cost	0.5 \$/kg waste
	Waste Disposal Cost	0.12 \$/kg waste

In Equation 3.14, cash inflow into the process is given by:

CF_i = Costs of all components in PROD stream. Using the flowrates and mass fractions given in Table 3.6,

$$CF_i = \sum_k w_k \sum_j m_j \times \text{cost}_j = [50 \times (1.0 \times 0.75)] = 60.5 \text{ \$/s} = 1908\text{M\$/yr and,}$$

CF_o = Costs of all components in FEED stream + utilities costs +waste related costs i.e.,

$$CF_o = \sum_k w_k \sum_j m_j \times \text{cost}_j + WR_c = [80 \times (1.0 \times 0.5) + 25 \times (0.5 + 0.12)] \qquad = 55.5 \text{ \$/s}$$

$$= 1750.25 \text{ M\$/yr}$$

Depreciation is calculated by Equation 3.13:

$$F_d = \frac{F_c - F_s}{N_y} = \frac{10000 - 2000}{5} = 1600$$

$TI = CF_i - CF_o - F_d$ = 1908-1750.25 -1.6E-3 = 157.75 M\$/yr

$NI = TI*(1-Tx)$ = 102.54 M\$/yr

Hence, $CF_n = NI + F_d = 102.54 + 1.6E-3$ =102.54 M\$/yr

NPV is calculated by Equation 3.12:

$$NPV = \sum_{n=0}^{N_y} \frac{CF_n}{(1+i_r)^n} \qquad 3.12$$

$$= \sum_{n=0}^{5} \frac{102.54}{1.1^n} = 388.7M\$/yr$$

Annual worth factor is calculated by Equation 3.15:

$$A_f = \frac{i_r(1+i_r)^{N_y}}{(1+i_r)^{N_y} - 1} \qquad 3.15$$

$$\text{i.e., } A_f = \frac{0.1 \times (1+0.1)^5}{(1+0.1)^5 - 1} = 0.267$$

AEP is calculated by Equation 3.11:

$$\begin{aligned} AEP &= NPV * A_f \\ &= 388.7\times10^6\times0.267 = 103.8M\$/yr \end{aligned} \qquad 3.11$$

Thus, the amount of profit gained by using the design described in Section 3.5.1 is 103.8 *M$/yr*. *AEP* can be used to compare this design with an alternate one, the better one being the design, which gives a higher value of *AEP*.

3.6 Summary

This Chapter has given quantitative analyses of profitability, environmental impact and controllability of chemical processes. The quantitative analyses were demonstrated with example calculations. This Chapter showed that complicated industrial processes can be easily evaluated for their operability with simple tools like the ones given in this chapter. This research does not claim that these are the best methods to do the analysis, but what should be gathered is the importance of doing this kind of an analysis and the simplicity with which it can be done.

Chapter 4

ANALYSIS OF CONTROLLABILITY MEASURES

This Chapter discusses the need for an alternate controllability measure to singular value analysis, which was used in this work. The Chapter also discusses the characteristics that a controllability measure should possess and then suggests some existing controllability measures for further exploration.

4.1 Introduction

Controllability is a measure of the ability of a process to easily reject any disturbances upsetting the system and to still be able to meet the set points. By definition controllability does not depend on the controller but on the plant itself (Morari, 1995). The design of the plant is a principal determinant of the controllability of the process. Thus, controllability considerations during design itself, play a major role in enhancing this ability of the system.

Many control systems have been developed that when installed and integrated with the process design, will try to smoothen the upsets and disturbances in the process. But these controllers are additional pieces of equipment added to an existing design of the process. Additional equipment means additional capital and maintenance expenditures, which any design engineer would like to avoid. So, control issues should be considered at the design stages itself. Seborg and coworkers (Seborg et al., 1989) illustrate with several examples how design affects process dynamics and control. Ziegler and Connell

(1994) demonstrated with several examples that minor changes in the process can improve controllability of the design by a large amount.

Ziegler and coworkers (1943), who are the pioneers in controllability, say that a poor controller may often perform acceptably on a process which is easily controlled, but the finest controller if used for a miserably designed process, might not deliver the desired performance. Along the same lines, a process that is very difficult to control with one control strategy may be easily controlled with another. So, controllability should be looked more from the design point of view than the control point of view.

The main idea behind studying controllability of a process is to see whether the process has the capacity to perform smoothly in the face of any disturbances, and not to test whether the control system installed is a good one or not. To assess the controllability of a process, a good controllability measure is required. The following section discusses the controllability measure used in this work and the reasons why a better controllability measure should be sought.

4.2 Singular Value Analysis

4.2.1 Overview of Singular Value Analysis

Singular value analysis is a tool used to analyze the overall control strategy of a multi-input multi-output system (MIMO). Singular value analysis helps in picking a good control strategy (combinations of controlled and manipulated variables). This tool develops the steady state gain matrix of the process, and then subjects the matrix to singular value decomposition to calculate the controllability index (condition number) of that design. This index can be used to compare alternate designs and select the best.

Singular value analysis has been chosen for this work to perform controllability analysis. The following section justifies the use of singular value analysis in this research.

4.2.2 Justification for Use of Singular Value Analysis

A control strategy is a set of combinations of *CV* and *MV*. A good combination of *CV* and *MV* is very significant in controlling the process. These strategies stem from the design of the process rather than that of the control system. As discussed in the previous sections, study of control should be started from the design stage itself, and in this, finding a suitable control strategy is a very good place to start. This is where the utility of singular value analysis comes into picture.

The focus of this work, as has already been stated, is to provide a method to evaluate a process design for its operability before being implemented in industry. Environmental impact (E), economic feasibility ($) and controllability studies have been used to rank alternatives, and though E and $ are appropriate for choosing between alternative designs, SVA has some limitations in choosing between alternatives based on controllability [1]. But, this tool is very useful for this study, as the individual capacities of each design to achieve controllability should be determined before they can be compared, which is exactly what singular value analysis does. SVA compares alternate control

[1] An important point to be noted is that SVA has been used for ranking alternatives in this work only after cross checking in literature that the tool has been used for similar purposes. Barton and coworkers (Barton et al., 1986) compare 11 floatation circuit designs with process condition number and proposed the best designs based on the condition number. They also prove that their results are accurate based on experimental set ups of control systems for the designs.

strategies for a process and selects the best. Overlooking this step might lead to a study where a set of designs, which are by nature uncontrollable, are compared and then the "best" of them is proposed. Also, Johnston and Barton (1987) proved that singular value analysis is a faster technique than dynamic simulation in assessing the performance of control strategies.

Hence, SVA can be considered as a preliminary tool in control studies. The step following the application of SVA should be to find a better tool for comparing alternatives, for which the tools that will be discussed in Section 4.4 may be explored. While exploring for better tools, the point to be conscious of is that a quantitative analysis (like measuring with condition numbers) alone is never sufficient to decide the better alternative. "Good Control" is difficult to define as that "goodness" depends on several factors, and hence finding a good measure for controllability is difficult. The decision should also be based on a subjective and qualitative analysis. This is where industrial experience plays a crucial role. This aspect will be discussed in detail in Chapter 7.

The following section describes the limitations that SVA suffers from, which necessitates the exploration for a better tool to measure controllability.

4.2.3 Limitations of Singular Value Analysis

Singular value analysis is constrained by some limitations, which makes it appear to be an inadequate tool for controllability analysis. Some limitations of SVA are:

- The first limitation that should be discussed is the assumption that singular value analysis makes. SVA assumes that a perfect controller has been installed in the system and any remaining controllability problems must be due to characteristics of the process (Johnston and Barton). But, a process with a real control scheme may behave quite differently to when a perfect controller is used.

- In singular value analysis, the singular values of the steady state gain matrix and the condition number are calculated. For good controllability, the requirement of SVA is that the singular value (σ) should be large and the condition number (*CN*) should be small. This requirement does not allow any relationship between σ and *CN* as the quantification measures of the process are just small and large (Narraway and Perkins, 1993). Hence, the tool is not very convenient to assess the controllability characteristics of individual designs.
- The main purpose of SVA is to assess the influence that the manipulated variables have on the controlled variables. Hence, the tool is more useful to compare alternate control strategies for the same process design rather than compare alternate process designs.

The limitations of SVA stated above convey the need to find a better tool to measure controllability. Before discussing existing controllability tools, the features that the alternative tool to measure controllability should possess, need to be studied. After studying these features, a tool which possesses these features should be explored for.

4.3 Alternative Controllability Measure

This section discusses the features that an alternative controllability measure should possess in order to be able to measure the controllability of a chemical process. As has been discussed in the previous sections, controllability should be studied from a design perspective rather than a control perspective. The features of the design play a crucial role in determining the controllability of the process.

The first part of this section (Section 4.3.1) discusses those features of a design that the controllability measure should be able to evaluate. The second section (Section 4.3.2) discusses the essential features that the controllability measure should possess in order to evaluate the design.

4.3.1 Controllability Features of a Design

Some of the features that a process design needs to possess for controllability are:

1. The process should allow easy manipulations.
2. Measurements of any process parameters should be noise free.
3. Manipulated variables (*MV*) should not exceed the degrees of freedom (*DOF*) (Seborg et al., 1989).

$$MV \leq \# DOF \tag{4. 1}$$

   This will ensure that there is sufficient number of variables that can be manipulated to achieve good control.

4. Every controlled variable should have at least one manipulated variable, which has a significant effect on the CV.

$$\# MV \geq \# CV \tag{4. 2}$$

   If criterion 4 is not satisfied, then there will be some *CV* left without a means to help them reach their set points.

5. The process should be insensitive to disturbances.
6. Manipulated variables should have a stronger influence on the process than the disturbance variables (*DV*). A steady state comparison of the influence of each variable on the process can be measured by Equation 4.3.

$$r = \frac{\dfrac{\Delta CV}{\Delta DV} DV_D}{\dfrac{\Delta CV}{\Delta MV} MV_D} \qquad 4.3$$

Here, Δ is the change in value of variable and D is the maximum acceptable deviation by which the variable can change. If $r \ll 1.0$, then the *MV* have a stronger influence on *CV* than *DV*. If *DV* have a stronger influence, then *CV* will be permanently deviated from their set points and control can never be achieved.

7. Equipment should be sufficiently sized to avoid operating on constraints.
8. The process should be designed to minimize transport delay, long lags and recycle.
9. The process should also be designed to minimize interactions between the manipulated and controlled variables. For example, MV_1 affects CV_1 but should not upset CV_2.
10. The time required to move to a new operating condition should be small.
11. The rate at which disturbances and process changes push a process away from desired operation should be slower than the rate at which the manipulated variable can return the process to the desired operation.

The eleven design criteria for controllability stated above appear to be very simple to test for, but are also very crucial as they determine the potential of the process to achieve the desired output. Another important observation that needs to be made here is that though all of the criteria determine the controllability of the process, a controller is not involved. The design of the process is what is being evaluated. This proves the point that the design of the process plays a major role in the controllability of the process.

4.3.2 Essential Features of a Controllability Measure

Following are the features that the controllability measure should possess to be able to evaluate the controllability of a design.

- The most essential feature of the measure for controllability is that, it should be capable of measuring all the controllability features of the process design, which were discussed in the previous section.
- Some of the controllability features discussed in Section 4.3.1 are difficult to quantify. So, the controllability measure should be capable of evaluating these features qualitatively and assess the potential of the design for controllability with respect to these "unmeasurable" features of the design.
- Since the controllability measure should take into account multiple criteria (controllability features that were discussed in the previous section), the measure should have the facility to take the aid of a multiple criteria decision making tool (See Appendix F).
- Depending on the decision maker's requirements and the design being studied, the controllability measure chosen should be either a steady state or a dynamic measure.

The following section discusses existing tools, which can be explored to design the alternative controllability measure.

4.4 Use of Existing Tools in Developing the Alternative Controllability Measure

A lot of work has been done on controllability since the pioneering work by Ziegler and Nichols (1943). Many attempts have been made to formulate a measure for controllability. Section 4.4.1 discusses the controllability measures that can be used with steady state information alone, and Section 4.4.2 discusses those measures that require dynamic information. Before going to the next section, what should be noted is that when ill-behaved dynamics or constraints are the primary control-related problems, dynamic models for control offer distinct advantages and when nonlinear or non-stationary effects are the primary control problems, steady state models can deliver similar advantages as the dynamic models with considerably less effort (Ramchandran, 1998).

4.4.1 Steady State Controllability Measures

A lot of literature has been published supporting steady state evaluation of controllability. Fisher and coworkers talk about steady state control as a prelude to dynamic control (Fisher et al., 1985b). Terrill and Douglas (1987b) write that steady state considerations alone can help in the identification of controllability limitations (like an inadequate number of manipulated variables to be able to satisfy process constraints and to optimize all the significant operating variables). Following are some of the steady state measures developed to measure controllability.

- Relative Gain Array, first introduced in 1966 by Bristol (1966): The relative gain array is a steady state interaction measure for multivariable control. This measure quantifies the effect of complete control of all controlled variables on the transfer function between a given manipulated variable and a given controlled variable.
- One major measure for controllability is economics (Fisher et al., 1988a; 1988b; 1988c). The better alternative is the one which has better economics. But, there

might be occasions when the situation demands a high expenditure in order to achieve good control.

- Singular value analysis (SVA) (Johnston and Barton ; Klema and Laub, 1980; Moore, 1986; Seborg et al., 1989): The main idea behind singular value analysis is to see how ill-conditioned the gain matrix of the system is. Ill-conditioning of the gain matrix reflects the bad choice of a control strategy. SVA was discussed in detail in Sections 3.2.2 and 4.2.
- Yi and Luyben (1995) used steady state disturbance analysis to screen alternative control structures. This analysis is a procedure in which the steady state variations of all variables are examined and evaluated for a given control structure when load disturbances occur.
- Weitz and Lewin (1996), and Naot and Lewin (1995) developed a simple procedure for screening flowsheets for controllability, which relies on the derivation of a simplified dynamic model using steady state flowsheet information.
- Lewin (1996) used 'disturbance cost' to quantify the required control effort to keep the control variables at the desired setpoint, which allowed the investigation of the effects of directionality in disturbances over a range of frequencies on the control quality utilizing a linearized process model.
- Seferlis and Grievink (1999) write that since the full count of all possible combinations between potential manipulated and controlled variables may be very large, use of dynamic simulations, singular values and interaction measures for the control quality may become prohibitive. Hence, they incorporate static controllability criteria in the early design of process systems and plantwide control systems. They

used a performance index to assess the ability of the different control structures to compensate for the effects of disturbances. This helped in the elimination of those control structures that have poor steady state disturbance rejection characteristics.

4.4.2 Dynamic Controllability Measures

Narraway and Perkins (1993) defines controllability analysis as that concept concerned with the dynamic characteristics of processes in the neighborhood of steady state operating point. In a series of papers, Belanger and Luyben (1998a; 1998b; 1998c), show that dynamic considerations at early stages of design can greatly increase the profitability of the plant. Following are some of the dynamic measures developed to measure controllability.

- Dynamic resiliency by Morari (1983a): Dynamic resiliency is concerned with the achievement of perfect control. Perfect control is possible only if the system transfer function matrix, $G(s)$, has a right inverse, $G^{-1}(s)$, i.e.,

$$G(s)\,G^{-1}(s) = I \qquad 4.4$$

- Time delays by Holt and Morari (1985): Since, time delays hamper the achievement of perfect control, Holt and Morari suggested a measure for assessing the controllability of multivariable time systems. For a system described by an m x m transfer function matrix, each measure is an m-vector of delay times.
- Functional controllability by Perkins and Wong (1985): Perkins and Wong followed up Holt and Morari's work (1985) and developed a scalar measure to assess the impact of delays on controllability. The source of such a measure is the theory of functional controllability. The idea underlying the theory is to investigate conditions under which a desired trajectory for the outputs from a plant may be specified, and

inputs found which generate the desired trajectory. A necessary and sufficient condition for functional controllability is also the invertibility of the transfer function matrix, $G(s)$.

- Economics: Narraway and coworkers (1991) propose a direct assessment of the impact of disturbances on system economics as a method of controllability analysis.
- Quality of control, Q, by Ziegler and Connell (1994a; 1994b): In a series of papers, Ziegler and Connell stress on the importance of process design in controllability and prove that minor changes in the process can improve the controllability by large amounts. They propose a controllability index called Quality of Control, Q, defined as:

$$Q = s / \tau \qquad 4.5$$

where, s = controller gain

τ = Period of oscillation, the inverse of recovery time from a load change.

Though a steady state evaluation is acceptable as a preliminary tool, a dynamic evaluation is required for a proper controllability analysis. But, unfortunately dynamic evaluation of controllability has not been very popular. The observations made by McAvoy and Belanger reflect the unchanged perceptions on dynamic analysis over the past two decades:

- In 1987, McAvoy says that no one readily available dynamic simulation package exists that facilitates analyzing process operability and control at the design (McAvoy, 1987).
- In 1998, Belanger writes that unfortunately, due to the current capabilities of simulation software, limitations in computer speed, the need to minimize engineering

man hours, and lack of adequate dynamic information for dynamic modeling, detailed dynamic studies during the conceptual design phase are not always practical (many engineers currently infer dynamic controllability from steady state information) (Belanger and Luyben, 1998a).

These observations make the prospects of conducting a dynamic analysis quite bleak. But, the developments in software, computer speeds, etc from the eighties to the nineties by itself should reflect the ability of the growing technology to be able to develop a tool that takes into consideration the dynamic aspects of controllability at the design stage in the near future.

4.5 Future Recommendations for Controllability Analysis

Based on the discussion in this chapter on controllability analysis, some recommendations can be made for future work in controllability analysis. The recommendations are:

- The effectiveness and practicability of the controllability measures, discussed in Section 4.4 should be explored further to determine which one(s) if any best suit the needs of the particular process.
- Narraway and Perkins (1993), in a critique of controllability measures, especially functional controllability and dynamic resilience, write that these controllability measures can be used to rank different processes with similar economics, but are not useful for those processes with differing economics. The reason for this drawback is that the controllability indicators generate indices of the quality of control attainable for the selected control structure, rather than indicating the performance of the control structure with respect to the process control objectives. Hence, an index of

performance that allows the estimation of value of control should be formulated. Ideally this index would be an economic performance indicator (Narraway and Perkins, 1993).

- If SVA is adopted, the user should be conscious of the fact that the analysis assumes a perfect controller to have been installed. When implemented on a real control scheme, the results could be significantly different.
- The development in technology should be taken advantage of and there should be more dynamic considerations in the development of the alternative controllability measure.
- To link conceptual process synthesis and plant wide control, there is a need to reduce as much as possible the potentially large number of control configurations through a rigorous screening (Schijndel and Pistikopoulos, 1999). For this, advances in thermodynamic and phenomena based representations for process synthesis and process control need to be studied.

4.6 Summary

This chapter discussed the attributes and limitations of singular value analysis. Section 4.3 discussed the need and features required of an alternate controllability measure. The design criteria for controllability and the various controllability measures available to quantify the controllability of a chemical process have been studied. The reasons why control issues should be considered at the design stage itself were discussed.

From these discussions, what can be observed is that the interaction between design and control is very crucial for achieving controllability. This interaction between design and control has been a very popular concept. Ziegler (1994a; 1994b) (the pioneer in controllability studies) stressed on the importance of process modifications, rather than controls modifications, to achieve good control. Thus, an important observation to be made is that controllability studies start from the design of the process itself and many problems associated with control can be tackled at the design stage itself.

Chapter 5

HOT AND COLD WATER MIXING SYTEM

In this Chapter, the coding and testing of singular value analysis used for controllability analysis is studied. The first system chosen for testing the methodology developed for controllability analysis in Chapter 3 is a simple system of hot and cold water mixing. This system is taken from Dr. Moores work (Moore, 1986). The system is simulated in ASPEN PLUS™. The simple mixer block in Aspen Plus™ is chosen for the mixer. This code is used as a template to develop the same for the second case study, manufacture of methyl chloride by hydrochlorination of methanol (See Chapter 6).

5.1 System

A hot water stream and a cold water stream flow separately into a mixer. The flow sheet is shown in Figure 5.1. The temperature of the mixture reaches an equilibrium and the fluid flows out. Thus, there are two inlet streams, hot and cold water, and one outlet stream, the product stream. The temperatures and flow rates of all three streams are monitored. The input values of the hot and cold water streams are as follows:

Flow rate of cold water (F_{CO}) = 20gpm = 0.0015m^3/s

Flow rate of hot water (F_{HO}) = 10gpm = 0.00075m^3/s

Temperature of cold water (T_{CO}) = 291 K

Temperature of hot water (T_{HO}) = 311 K

When this system was run is ASPEN PLUS™, the following steady state optimum values are obtained for the mixture:

Flow rate of mixture (F_{MO}) = $0.00225 m^3/s$

Temperature of mixture (T_{MO}) = 298 K

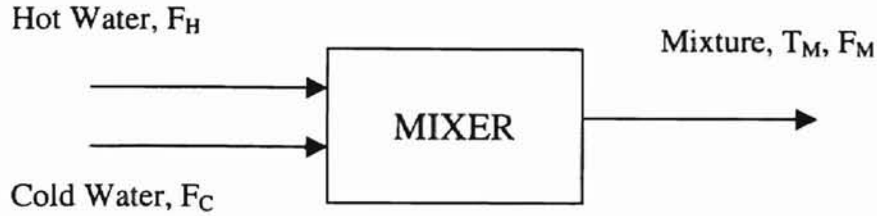


Figure 5. 1 Flowsheet for Hot and Cold Water Mixing System

5.2 Controllability Analysis (Singular Value Analysis, SVA)

Singular Value Analysis has been discussed extensively in the previous two chapters. Chapter 3 presented the description of SVA and its methodology. The reasons for choosing SVA, despite the limitations that it suffers from, have been given in Chapter 4. In SVA, a control strategy is chosen and the steady state gain matrix of that system is developed. Then the singular values for that matrix are calculated. Based on the singular values, a controllability index called ***Condition Number*** is calculated. Alternate control strategies are designed and the condition number is used to compare these strategies. The strategy having the lowest condition number is chosen as the best control strategy for the corresponding design.

Steady state gain is defined as the ratio of the deviation of output variable to that of the input variable; or the ratio of the deviation of the controlled variable to that of the manipulated variable. See Equation 3.4.

$$K_{ij} = \frac{(CV_i - CV_{iO}) / CV_D}{(MV_j - MV_{jO}) / MV_D} \qquad 3.4$$

The elements, K_{ij}, form the steady state gain matrix.

In the hot and cold water system, the temperature and flow rate of the product stream are to be controlled. These variables are controlled by using the flow rates of the hot and cold water streams as the manipulated variables.

5.2.1 Variables in the Hot and Cold Water System

Following are the manipulated and controlled variables required to build the steady state gain matrix (See Section 5.2.2) of the hot and cold water system:

Manipulated Variables (MV): Flow rate of cold water stream, F_C (kg/s)

Flow rate of hot water stream, F_H (kg/s)

Controlled Variables (CV): Temperature of mixture stream, T_M (K)

Flow rate of cold water stream, F_M (kg/s)

5.2.2 Development of the Steady State Gain Matrix for the Hot and Cold Water System

Section 3.2.2 describes the method by which a steady state gain matrix is developed. In this section the gain matrix is developed for the hot and cold water system. The pairing of the MV and CV is as follows:

F_C --- T_M, i.e., F_C controls T_M

F_H --- F_M, i.e., F_H controls F_M

Using Equation 3.4, the steady state gain matrix is developed in the same manner as shown in Table 3.1. Specific to the hot and cold water system the matrix appears as shown in Table 5.1.

Table 5. 1 Steady State Gain matrix for the Hot and Cold Water System

	$F_C(MV_1)$	$F_H(MV_2)$
$T_M(CV_1)$	K_{11}	K_{12}
$F_M(CV_2)$	K_{21}	K_{22}

The singular value analysis is done in ASPEN PLUS™ with the help of its USER unit operation model. The flowsheet of the hot and cold water system has been modified in Aspen to accommodate the User block (See Figure A.1). The code for SVA was inserted in the User model. The value of the first manipulated variable, F_C, was changed by 10% and the changes in T_M and F_M were noted down. Then F_H was changed by 10% and again the changes in T_M and F_M were noted down. The gain matrix was developed as described in Chapter 3. The matrix was then subjected to singular value analysis and the condition number for the strategy was calculated by the ratio of the maximum singular value to the minimum singular value or, Equation 3.5,

$$CN = \sigma_1 / \sigma_r \qquad 3.5$$

The strategy with the lowest CN is the best.

Alternate control strategies were designed by varying the amount of change that the MV was subjected to. As mentioned earlier, in the first strategy, MV is changed by 10%. Now, in the second strategy, MV is changed by 1% and in the third one by 0.1%. In this manner three control strategies were designed, and the *CN* for each was evaluated in ASPEN. The results are as shown in Table 5.2. The results in Table 5.2 show that, CN increases as the change in MV increases, which can be expected logically as a large change in the value of MV would make the process more difficult to control. This

Table 5. 2 SVA Results for the Hot and Cold Water System

S.No.	Percentage Change in *MV*	*CN*
1	10	178.7678
2	1	38.4871
3	0.1	38.2563

proves the utility of singular value analysis. So, amongst the three strategies designed, strategy 3 is the best as it has the lowest CN.

The simplicity of the hot and cold water system helped in developing the singular value analysis easily in ASPEN PLUS™. The user block model option in Aspen was used to code the entire analysis (See Appendix C). Again, the simplicity of the system made it inflexible to make alternate designs and compare them using the condition number. For this reason, another system, manufacture of methyl chloride by the hydrochlorination of methanol, was chosen to perform a more rigorous controllability analysis. This is dealt with in Chapter 6.

5.3 Summary

In this chapter, the singular value analysis has been tested on a simple hot and cold water mixing system. The code developed for the system (See Appendix C) is used as a template to develop the code specific to the methyl chloride process (See Chapter 6 and Appendix D). Since environmental impact and economic feasibility analyses are more straight forward, they were tested directly on the methyl chloride process (See Chapter 6) and not conducted for the hot and cold water system.

Chapter 6

METHYL CHLORIDE PROCESS

Chapter 3 discussed measures for quantifying controllability, environmental impact and profitability. Singular value analysis, used for controllability measurement, was tested and implemented on the hot and cold water system (See Chapter 5). In this Chapter the code developed for SVA for the hot and cold water system is tested on a second case study, manufacture of methyl chloride by the hydrochlorination of methanol. This system was taken from the work of Dantus (1995). Also, measures for environmental impact and profitability developed in Chapter 3 are used to evaluate the methyl chloride process.

6.1 Introduction

Methyl Chloride is a colorless gas with a mild odor and a sweet taste (Dantus, 1995). A major portion of the production of methyl chloride is used in the production of silicones. The demand for methyl chloride has risen from 650 to 670 million pounds from 1996 to 1997 respectively, and is projected to rise to 775 million pounds by 2001 (CMR, 1997). The use of methyl chlorosilanes as intermediates for the production of silicones has been increasing at an annual rate of about 2.5 to 3% over the past decade. These uses of methyl chloride was a good motivation to use the system as the second case to apply and test the developed methodologies for evaluating operability criteria.

6.2 Modifications to the Original Methyl Chloride Process

A major portion of this work is on the study of controllability. The singular value analysis used for the evaluation of the controllability of the process, as described in Chapters 3 and 4, mainly determines the interaction between various variables governing the process. For this reason, the original process (See Figure 6.1) borrowed from the work of Dantus (1995) had to be modified to accommodate the requirements of the controllability analysis being conducted in this research.

One major modification was that the recycle loop was removed. Only one liquid product is taken out from the bottom of the flash chamber now, thus avoiding the separation of unreacted feed and recycling. The vapor product from the flash chamber is sent to a separator as earlier and this vapor is separated into the main product, methyl chloride and waste, which contains the unreacted feed and water.

Another modification was that two heat streams were added to the design of the process. These heat streams could be manipulated easily to control the product purity and flow rate (See Section 6.5). The new chemistry proposed, i.e., hydrochlorination of methanol to give methyl chloride was retained. As discussed in Chapter 1, this chemistry was chosen as it is the commercial mode of production, and also, hydrochlorination of methanol has been proved to be a better chemistry for environmental studies than thermal chlorination of methane (Dantus, 1995). The new design is shown in Figure 6.2.

6.3 Initial Steady State Optimum System

The process chosen for this work is the manufacture of methyl chloride by the hydrchlorination of methanol. As discussed in the previous sections, the system chosen

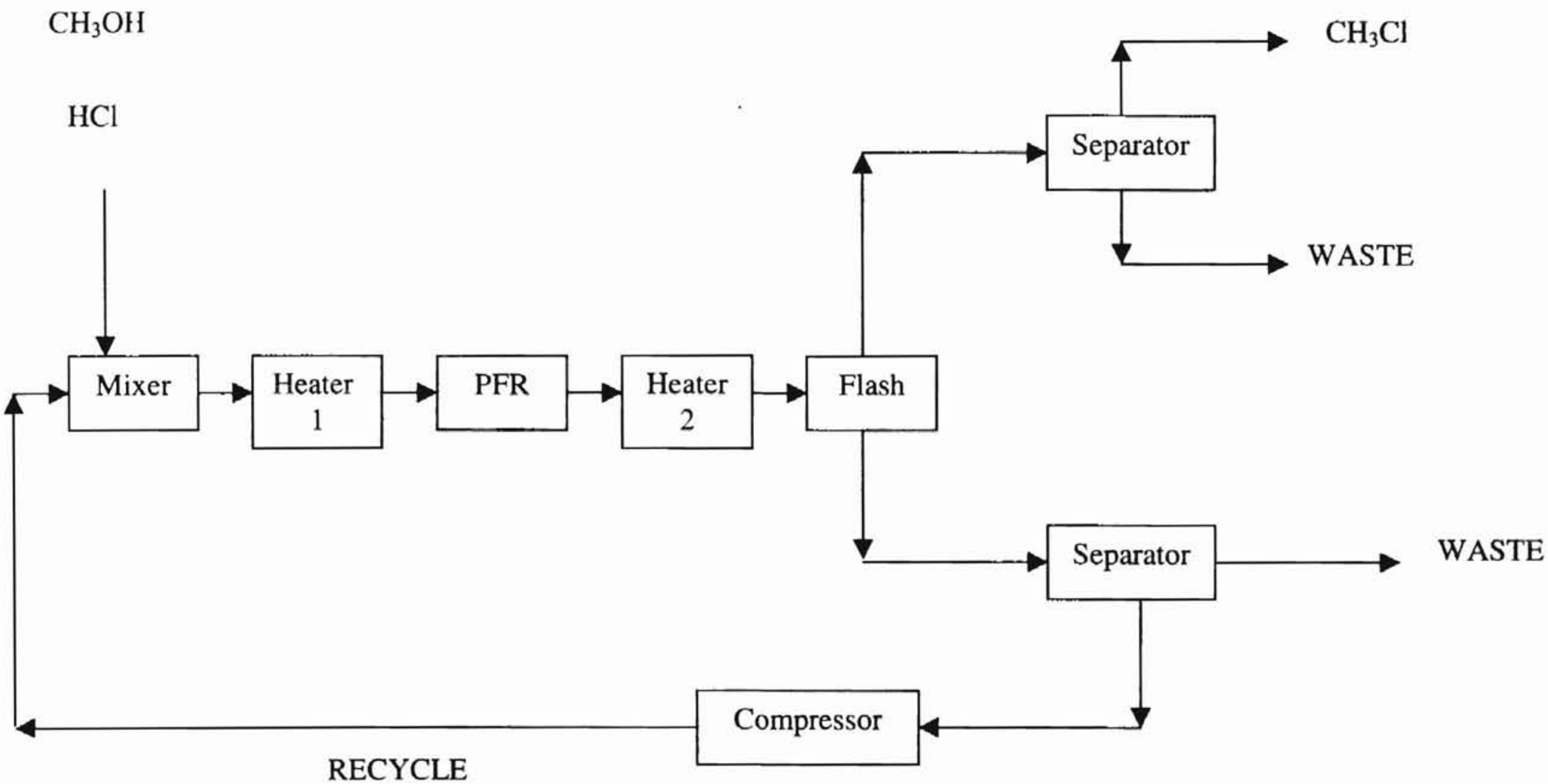


Figure 6. 1 Original Flowsheet for the Methyl Chloride Process (Dantus, 1995)

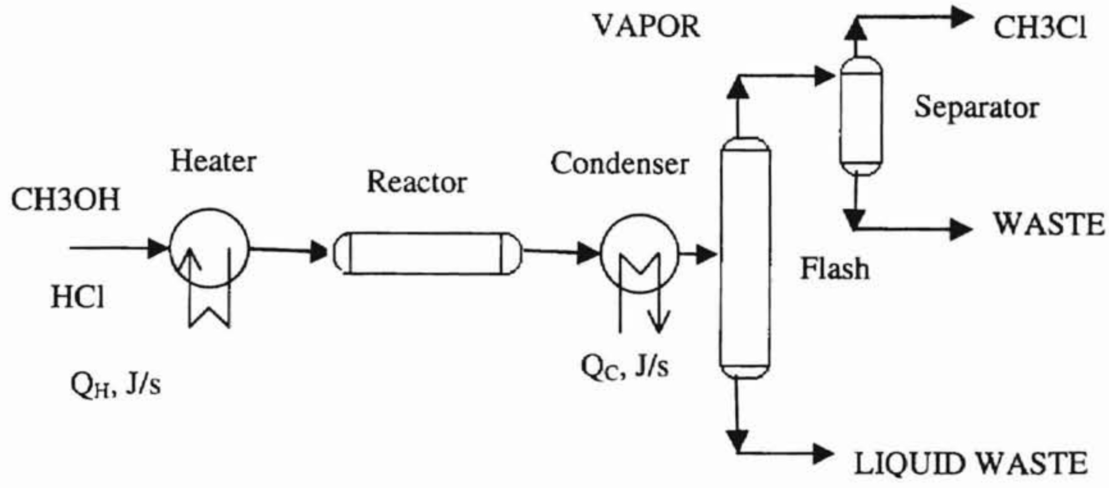


Figure 6. 2 Modified Flowsheet for the Methyl Chloride Process

for this work has been borrowed from the work of Dantus (1995). Dantus started with a base case, and then designed seven alternates to the base case. He compared the base case and the seven alternate designs with respect to the impact of each on the environment. The result of this comparison was that a final optimum design, which had the least effect on environment, was proposed.

Since this final optimum design has been proved to be environmentally friendly, it was chosen for the current research (after some modifications have been made in the manner described in Section 6.2) as the initial design (or Alternate 1) to now check for the process's operability and profitability following the motivation described in Section 1.4 (See Figure 1.1). The initial optimum system (Alternate 1) is described below.

The chemistry used for the designs is the hydrochlorination of methanol to give methyl chloride. This is given by the following equation:

$$CH_3OH + HCl \rightarrow CH_3Cl + H_2O$$

Temperature to which the mixture of CH_3OH and HCl are heated before entering the reactor = 644 K.

Pressure of the mixture = 1 atm.

Flow rate of HCl = 20 gmol/s

Flow rate of CH_3OH = 20 gmol/s

Product flow rate (CH_3Cl) desired = 12.5gmol/s

The following section discusses the alternate designs to the initial steady state optimum design of the methyl chloride process.

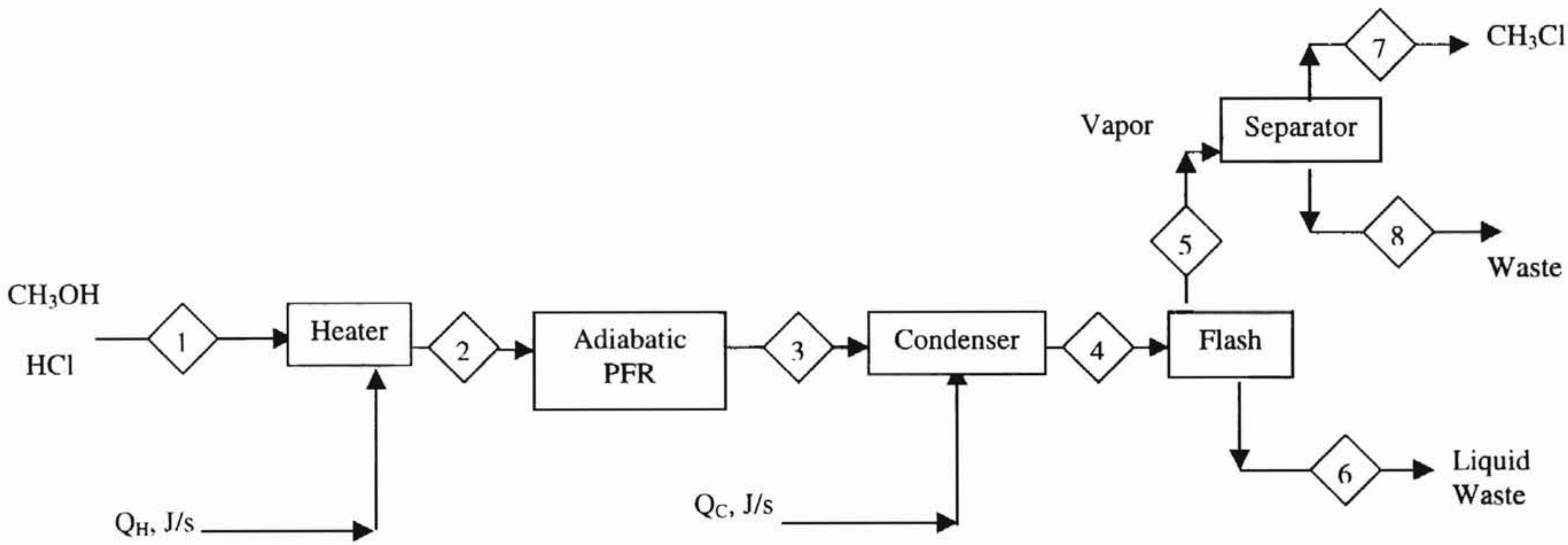
6.4 Alternate Designs for the Methyl Chloride Process

Section 6.3 describes the process chosen for this work. The main objective of this research (See Section 1.1) is to compare alternative process designs and select the design that is best feasible and operable. Hence, for that reason alternate designs to the initial steady state optimum design have been prepared. The initial optimum design is treated as Alternate 1 as this is a continuation of Dantus (1995) work and not a process that the current research work originally started with.

As described in the previous section, the initial optimum system or Alternate 1 uses an adiabatic PFR. Two alternates to this design have been prepared. The two alternate designs are:

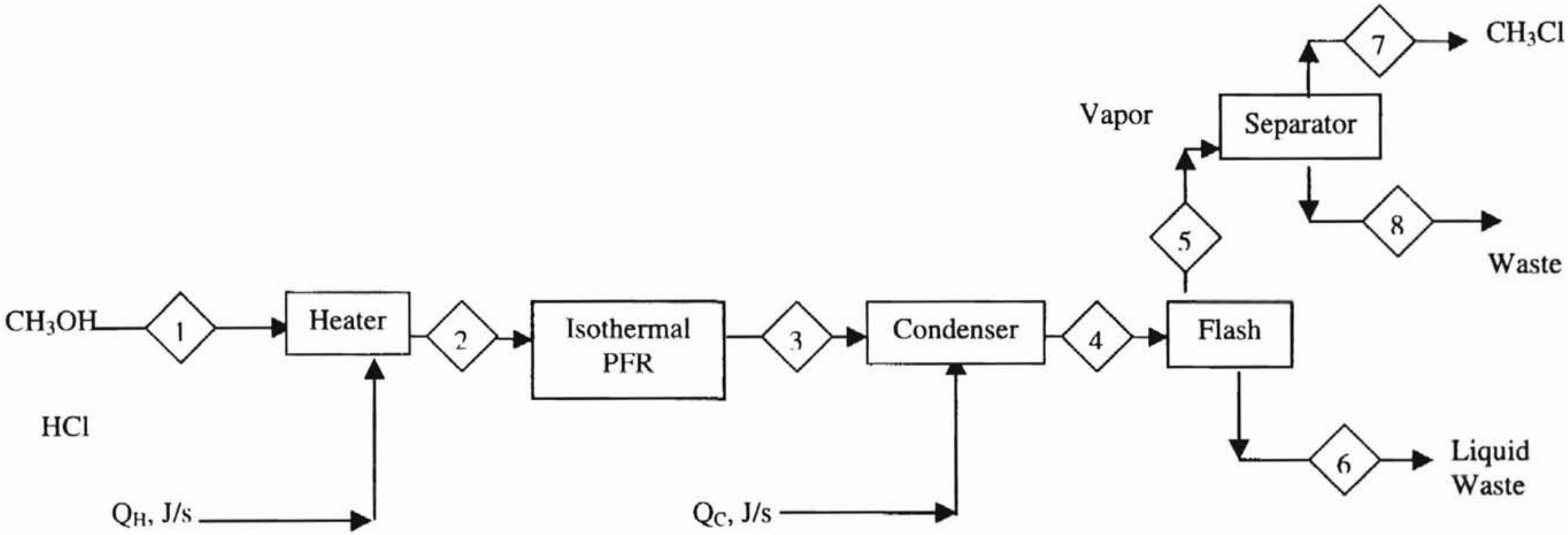
- Alternate2: Uses an isothermal PFR instead of the adiabatic PFR in Alternate 1.
- Alternate 3: Uses an isothermal CSTR instead of the adiabatic PFR in Alternate 1.

The process flow diagrams (PFD) for the steady state simulations of the three alternates are given in Figures 6.3, 6.4 and 6.5 respectively. The three alternates are compared with respect to C, E and $. The evaluation of the three criteria and comparison of the



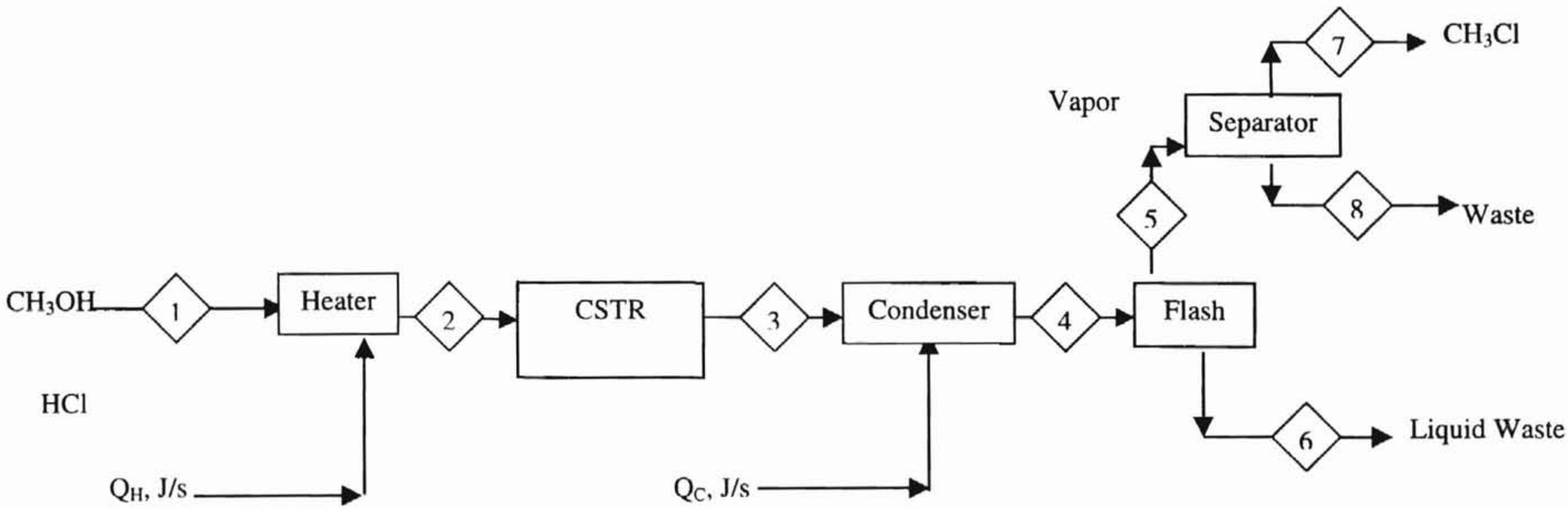
Stream #	1	2	3	4	5	6	7	8
Temperature (K)	300	640	842	346.5	374	374	374	374
Pressure (Atm)	1.0	1.0	1.0	1.0	2.9	2.9	2.9	2.9
Vapor Fraction	0.59	1.0	1.0	0.97	1.0	0.0	1.0	0.0
Mass Flow (kg/s)	1.37	1.37	1.37	1.37	1.324	0.047	0.63	0.69
Mole flow (gmol/s)	40.0	40.0	40.0	40.0	37.85	2.15	12.5	25.35
Enthalpy (J/gmol)	-1.62E5	-1.32E5	-1.32E5	-1.57E5	-1.51E5	-2.64E5	-0.83E5	-1.98E5
Component mole flow (gmol/s)								
CH_3OH (gmol/s)	20.0	20.0	7.4	7.4	7.07	0.33	0.0	7.07
HCl (gmol/s)	20.0	20.0	7.4	7.4	7.4	0.019	0.0	7.4
CH_3Cl (gmol/s)	0.0	0.0	12.6	12.6	12.5	0.087	12.5	0.0125
H_2O (gmol/s)	0.0	0.0	12.6	12.6	10.9	1.72	0.0	10.9

Figure 6. 3 Process Flow Diagram for Methyl Chloride Process, Alternate 1 (uses Adiabatic PFR)



Stream #	1	2	3	4	5	6	7	8
Temperature (K)	300	842.8	842.8	344	374	374	374	374
Pressure (Atm)	1.0	1.0	1.0	1.0	3.27	3.27	3.27	3.27
Vapor Fraction	0.59	1.0	1.0	0.74	1.0	0.0	1.0	0.0
Mass Flow (kg/s)	0.99	0.99	0.99	0.99	0.81	0.186	0.63	0.176
Mole flow (gmol/s)	29.0	29.0	29.0	29.0	20.3	8.7	12.51	7.8
Enthalpy (J/gmol)	-1.62E5	-1.2E5	-1.37E5	-1.7E5	-1.32E5	-2.62E5	-0.83E5	-2.4E5
Component mole flow (gmol/s)								
CH_3OH (gmol/s)	14.5	14.5	1.24	1.24	1.22	0.35	0.0	0.89
HCl (gmol/s)	14.5	14.5	1.24	1.24	1.22	0.027	0.0	1.22
CH_3Cl (gmol/s)	0.0	0.0	13.26	13.26	12.52	0.735	12.51	0.0125
H_2O (gmol/s)	0.0	0.0	13.26	13.26	5.66	7.6	0.0	5.66

Figure 6. 4 Process Flow Diagram for Methyl Chloride Process, Alternate 2 (uses Isothermal PFR)



Stream #	1	2	3	4	5	6	7	8
Temperature (K)	300	842.8	842.8	346	374	374	374	374
Pressure (Atm)	1.0	1.0	1.0	1.0	2.96	2.96	2.96	2.96
Vapor Fraction	0.59	1.0	1.0	0.90	1.0	0.0	1.0	0.0
Mass Flow (kg/s)	1.23	1.23	1.23	1.23	1.13	0.10	0.63	0.50
Mole flow (gmol/s)	35.85	35.85	35.85	35.85	31.26	4.59	12.51	18.75
Enthalpy (J/gmol)	-1.62E5	-1.2E5	-1.34E5	-1.62E5	-1.47E5	-2.64E5	-0.83E5	-2.05E5
Component mole flow (gmol/s)								
CH_3OH (gmol/s)	18.0	18.0	5.25	5.25	4.68	0.57	0.0	4.68
HCl (gmol/s)	17.85	17.85	5.1	5.1	5.07	0.035	0.0	5.07
CH_3Cl (gmol/s)	0.0	0.0	12.75	12.75	12.52	0.23	12.51	0.0125
H_2O (gmol/s)	0.0	0.0	12.75	12.75	9.0	3.76	0.0	9.0

Figure 6. 5 Process Flow Diagram for Methyl Chloride Process, Alternate 3 (uses Isothermal CSTR)

alternate designs is given in the following sections. The calculations follow the same procedure as demonstrated in the example problem in Section 3.5. The present work uses the unit operation model, USER2, in ASPEN PLUS™ to develop the methodologies (See Figures A.2, A.3 and A.4). The steps to follow to conduct the analyses in ASPEN PLUS™ are explained in Appendix A.

6.5 Controllability

The code that was developed for the hot and cold water mixing system was used as a template to conduct singular value analysis for the methyl chloride process. Necessary changes that need to be made to suit the methyl chloride process were made. In this process, methyl chloride, i.e., product flow rate and product purity need to be controlled. These are controlled by using feed flow rate (*FEED*) and, heat to the reactor (*HEATH*) in one control strategy and heat to the condenser (*HEATC*) in another control strategy as the manipulated variables[1]. Thus, CV and MV for the system are:

Controlled Variables:

Methyl Chloride flowrate (*PROD*)

Product purity (*XPRD*)

Manipulated Variables:

Feed flow rate (*FEED*)

Heat supply to heater (*HEATH*)

Heat supply to condenser (*HEATC*)

[1] In the modified methyl chloride process, shown in Figure 6.2, the heat to the reactor or the heat to the condenser are supplied through a heater, and this heat is in turn supplied by a heat stream. Hence, the heat supply through the respective heat streams is the manipulated variable (MV2) for the corresponding control strategy.

The first strategy (Strategy 1), i.e., the combination of CV-MV chosen is *PROD-FEED* and *XPRD-HEATH*. The steady state gain matrix is developed in the same manner as in Section 3.2.2. A change is made in *FEED* (MV_1) and the changes in *PROD* (CV_1) and *XPRD* (CV_2) are recorded. Then a change is made in *HEATH* (MV_2) and again, the changes in CV are recorded. The steady state gain matrix was developed for this combination of CV and MV and is shown in Table 6.1.

Table 6.1 Steady State Gain Matrix for the Methyl Chloride Process with Strategy 1

	FEED (MV_1)	*HEATH* (MV_2)
PROD (CV_1)	K_{11}	K_{12}
XPRD (CV_2)	K_{21}	K_{22}

This matrix was then subjected to singular value analysis and the condition number for the matrix and, hence the control strategy was calculated. An alternate control strategy was designed by changing MV2 from heat supply to heater (*HEATH*) to heat supply to condenser (*HEATC*) i.e., the new strategy is: *PROD-FEED* and *XPRD-HEATC*. Table 6.2 shows the gain matrix for strategy 2.

Table 6.2 Steady State Gain Matrix for the Methyl Chloride Process with Strategy 2

	FEED (MV_1)	*HEATC* (MV_2)
PROD (CV_1)	K_{11}	K_{12}
XPRD (CV_2)	K_{21}	K_{22}

As discussed in Section 6.4, alternate designs are prepared by substituting the adiabatic PFR with an isothermal PFR (Alternate 2) and then a CSTR (Alternate 3). The isothermal PFR and the CSTR are operated at the exit temperature of the adiabatic PFR. (See Figures 6.3, 6.4 and 6.5). The results for the three alternates are given in Table 6.3.

Table 6. 3 SVA Results for the Methyl Chloride Process

Control Strategy (CV-MV Combination*)	Adiabatic PFR (Alternate 1)	Isothermal PFR (Alternate 2)	CSTR (Alternate 3)
1 (*PROD-FEED* and *XPRD-HEATH*)	25.4	33.7	8.2
2 (*PROD-FEED* and *XPRD-HEATC*)	38.2	3.6	2.5

* See previous section for details on the CV-MV combinations.

The results given in Table 6.3 show that for both strategy 1 and strategy 2 CSTR is more controllable than the other two alternates, as this alternate has the lower condition number (from Chapter 3, the lower the condition number, the better controllable is the strategy).

Another observation that can be made from the results in Table 6.3 is that when the control strategy is changed from strategy 1 to 2, the two designs with isothermal reactors (Alternates 2 and 3) show a drastic decrease in condition number whereas the adiabatic reactor (Alternate1) shows an increase, and hence becomes more uncontrollable. As discussed earlier, in strategy 1, a change in heat supply to the feed preheater (which will change the enthalpy entering the reactor) is made while in strategy 2, a change is made in the heat supply to the condenser which cools the product from the reactor (See Figure 6.2). Thus, the conclusion that can be drawn from these results is that the isothermal reactors are more sensitive to changes in heat supply to them (which makes them uncontrollable) than the adiabatic reactor.

6.6 Environmental Impact

As described in Chapter 3, environmental impact was calculated by estimating the impact of each chemical in each stream on the environment (See sample calculation in Section B.1). Thus, the streams that need to be considered are the feed stream, the effluent stream from the reactor, the vapor and liquid streams from the flash chamber, the product stream from the separator, which contains the final product and the waste stream from the separator (See Figure A.3).

The environmental impact indices of all the chemicals are calculated using equations 3.6 to 3.10 and standard data from the referred EPA documents (Davis et al., 1994; Bouwes and Hassur, 1997a; Bouwes and Hassur, 1997b). The calculated values of the indices are shown in Table 6.4.

Table 6.4 Environmental Impact Indices (ϕ_j) of Chemicals in the Methyl Chloride Process

S. No.	Chemical	Environmental Impact Index, ϕ_j (EIU/kg)
1	CH_3OH	15.48
2	HCl	77.1
3	CH_3Cl	25.4
4	H_2O	0.0

The equation required to calculate environmental impact of the methyl chloride process (Equation 3.6) along with the calculated environmental impact indices (Table

6.4) are incorporated into the USER block. First, the simulation is run at initial steady state optimum conditions. The resulting values of the environmental impact are shown in Table 6.5.

Table 6. 5 Comparison of Environmental Impacts of Alternate Designs of the Methyl Chloride Process

Alternate Designs	Environmental Impact, *E* (EIU/kg)
Adiabatic PFR (Alternate 1)	362.0
Isothermal PFR (Alternate 2)	207.8
CSTR (Alternate 3)	303.5

The results in Table 6.5 show that the design with the isothermal PFR (alternate 2) has least effect on environment, or in other words alternate 2 is the most environmentally friendly. Next, a combined controllability and environmental impact analysis is done on the system. In this combined analysis, calculations for both C and E are done together to observe if the incorporation of control strategies affects the values of *E*. The analysis is done by making a change of 1% in each multiplication factors of the manipulated variables individually, and utilizing control strategies 1 and 2 respectively (See Section 6.5). The change in the values of environmental impact for these two cases are given for the adiabatic PFR (Alternate 1) in Table 6.6.

The results in Table 6.6 show that the environmental impact reduces by a large amount when control strategy 1 is used and there is no change when control strategy 2 is used. The reason for this is that, with the first control strategy, heat supply to the reactor changes, as a result of which, the amounts of products generated in the product or waste streams varies. Hence, there is a difference in the environmental impact value (as E is a function of the mass of chemicals in a stream; See Equation 3.6). But, when the second control strategy is used, the heat supply to the condenser is varied, which varies the distribution of the products between the product and waste streams, but

Table 6. 6 Effect of Control Strategies on Environmental Impact for Adiabatic PFR (Alternate 1)

Control Strategy (CV-MV Combination*)	Change in Environmental Impact from Initial Optimum, *E* (EIU/kg)
1 (*PROD-FEED* and *XPRD-HEATH*)	362.0 to 287.5
2 (*PROD-FEED* and *XPRD-HEATC)*	362.0 to 362.0

* See Section 6.5 for details on the CV-MV combinations.

does not change the amounts of products generated. Hence, there is no variation in the environmental impact value[2]. The same procedure is repeated for the remaining two designs that use an isothermal plug flow reactor (Alternate 2) and a CSTR (Alternate 3) respectively. There was no variation observed in the environmental impact values from one strategy to the other for both the alternates.

This section, with the results in Table 6.5, have shown that comparing alternate designs for their environmental impact is very simple and the most environmental friendly design can be easily determined and selected. Also, results in Table 6.6 show

[2] The release factor, r, (See Equation 3.6) which determines the potential of the stream to release waste into the environment , has been taken as 1.0 for all streams for this research. If r was assigned the exact release potential value for each stream, there would probably have been a difference in the environmental impact values even when control strategy 2 is used. This is because the release factor would have been higher for

that environmental impact can be reduced by incorporating control strategies in the design of the process.

6.7 Profitability

Profitability ($) of the methyl chloride process is calculated as discussed in Section 3.4 (See sample calculation for Alternate 1 in Section B. 2). The expressions required for the calculation of $ are Equations 3.11 to 3.17.

The raw material costs, the utilities costs and the waste related costs are given in Table 6.7.

Table 6. 7 Economic Data for the Methyl Chloride Process

Cost		Cost
Chemical Costs	CH_3OH	0.101$/kg
	HCl	0.14 $/kg
	CH_3Cl	0.847 $/kg
	H_2O	0.00044 $/kg
Utilities costs	Feed Preheating	3.03E-9 $/J
	Cooling Water	7.3E-5 $/kg
Waste related costs	Treatment	1.1 $/kg organic mass
	Disposal	0.165 $/kg waste
Capital Cost		$19500

the waste streams, and the more the product in the waste streams, the higher would be the environmental impact of that particlar design.

Following the discussion in Chapter 3,

Cash inflow (C_i) = sum of costs of products, i.e., CH_3Cl and H_2O.

Cash outflow (C_o) = Raw material costs + utilities cost + waste treatment cost + waste disposal cost

The interest rate (i_r) is taken to be 10% and tax rate, 35% (White, 1998).

So, the information required to be sent to the User block is that of the feed stream the product stream, waste streams and the heat streams (See Figure A.4). The data from Table 6.7 were inserted into the input file (See Section D.1). Using the data from Table 6.7, and the expressions given in Chapter 3 (Equations 3.11 to 3.17), *AEP* was calculated for alternate 1. The same procedure was repeated for other alternates too. As for environmental impact, the simulation was first run at initial steady state optimum conditions. Results obtained are given in Table 6.8.

The results in Table 6.8 show that Alternate 2 with the isothermal PFR is the most profitable one, and Alternate 3 with the CSTR is the least profitable one. This is due to the large difference in the waste treatment and disposal costs, as shown in Table 6.8. Also, the PFDs of the three alternates (Figures 6.3, 6.4 and 6.5) show that Alternates 1 and 3 have more waste generated than Alternate 2. Hence, their waste related costs are higher.

Similar to the calculations in Section 6.6 for environmental impact, a combined controllability and profitability analysis is performed by changing each manipulated variable by 1% individually and observing the change in the profitability values from the initial steady state optimum values. The results are shown in Table 6.9.

Table 6. 8 Comparison of Profitability of Alternate Designs of the Methyl Chloride Process

End of Project	Adiabatic PFR (Alternate 1)	Isothermal PFR (Alternate 2)	Isothermal CSTR (Alternate 3)
Product Revenue (M$/yr)	16.87	16.87	16.87
Net Revenue (M$/yr)	16.87	16.87	16.87
- Raw Material Costs (M$/yr)	5.26	3.814	4.71
- Utilities Costs (M$/yr)	0.117	0.115	0.142
- Waste Treatment Costs (M$/yr)	3.81	1.22	6.25
- Waste Disposal Costs (M$/yr)	3.85	1.88	3.1
- Depreciation (M$/yr)	3.9E-3	3.9E-3	3.9E-3
- Write-off (M$/yr)	0.0	0.0	0.0
Taxable Income (M$/yr)	3.82	9.84	2.66
- Tax @ 35% (M$/yr)	1.34	3.44	0.932
Net Income (M$/yr)	2.48	6.39	1.73
+ Depreciation (M$/yr)	3.9E-3	3.9E-3	3.9E-3
+ Write-off (M$/yr)	0.0	0.0	0.0
Working Capital (M$)	2.9E-3	2.9E-3	2.9E-3
Capital Equipment (M$)	1.95E-2	1.95E-2	1.95E-2
Cash Flow (M$/yr)	2.49	6.4	1.73
NPV (M$/yr)	9.41	24.23	6.55
AEP (M$/yr)	2.48	6.39	1.73

The results in Table 6.9 show that strategy 1 has substantially increased the profits. In strategy 1 the heat supply to the feed preheater is changed (increased in this case). Thus, this change increased the products and reduced waste, which has lead to an increase in the profits. Thus, the apparent conclusion from this observation is that, incorporating the control strategy into Alternate 1 has two benefits: 1) It restores controllability to the process and, 2) It increases profits. When Alternates 2 and 3 were subjected to the same combined $ and C analysis, with the first strategy there was nodifference in results, but with the second one there was a slight decrease in profits, though Alternate 2 still continued to be the most profitable amongst the three.

Table 6. 9 Effect of Changing Control Strategies on Profitability for Adiabatic PFR (Alternate 1)

Control Strategy (CV-MV Combination*)	Change in Profitability from Initial Optimum, $ ($/yr)
1 (*PROD-FEED* and *XPRD-HEATH*)	2.48M to 5.42M
2 (*PROD-FEED* and *XPRD-HEATC*)	2.48M to 2.47M

* See Section 6.5 for details on the CV-MV combinations.

6.8 Summary

This Chapter showed the testing of the code developed (See Appendix D) for performing controllability, environmental impact and profitability analyses calculations on the methyl chloride process. Again, the simple calculations illustrated the ease with which this kind of operability study can be conducted and confirmed that a similar study can be easily done in industry. The effect of incorporating control strategies to restore controllability on the environmental impact and profitability of the methyl chloride process has also been studied.

Chapter 7

INPUT FROM INDUSTRY

A survey on the operability studies performed in seventy five industries has been conducted as a part of this research. This Chapter discusses the questions posed to the industrialists. About 28% of the companies responded and these responses of the industries to those questions are also discussed. This survey gave a sharper focus to the research.

7.1 Introduction

Feasibility and Operability imply the ability of a process to operate in an environmentally friendly, economically feasible and practical manner at any operating conditions. A measure of operability of a chemical process reflects the ability of the process to function smoothly in industry. The initial criteria that any process should satisfy to be deemed feasible and operable were listed as:

- Profitability
- Environmental Impact
- Controllability
- Resiliency
- Flexibility
- Safety

The main focus of this work has been to stress on the point that industry should ensure that their process achieves the best of all the criteria listed above to achieve results acceptable to society as well as to them. If the criteria are not satisfied in a favorable manner, progress of industry would be deterred and might eventually bring losses to them.

The ideas and opinions that have been expressed so far have been from a pure academic point of view. They have been gathered from literature and personal insight into the area of process operations. The extensive study in the area has lead the research to a conclusion that a violation of any of these criteria would bring losses to the industry and that every measure and precaution should be taken to meet them.

In order to make this research work more comprehensive, feedback from industrialists was sought on the issue of process operability. The motivation for seeking their opinion was that they are best capable of giving a very informative opinion in the context of real life processes. Based on their experience in industry, they certainly have a clearer picture of the intricacies of chemical processes and are capable of making a valuable contribution relevant to the current research. In this context a questionnaire was sent to 75 industrialists seeking their comments/suggestions/answers to some questions which are described in the next section. Responses were obtained from 28% of companies contacted. These responses are summarized in Section 7.3.

7.2 Questionnaire Sent to Industries

The questionnaire sent to industries was designed with the idea of improving operability studies and give a sharper focus to research in the operability area. Following are the questions posed to the industrialists.

1. Does your company do methodical evaluations of process designs for operability/controllability to guide process design at the PFD stage?
2. If yes, what are the criteria that you evaluate it upon, and what methods do you use to analyze the criteria?
3. If no, why don't you think it is necessary to evaluate the designs based on these criteria?
4. What criteria for operability/controllability do you think should be looked into to evaluate a process design?
5. What should academia do to provide you with an incentive to perform the operability/controllability analysis and evaluate process designs?

The responses to the above questions from the industrialists were varied and gave a new perspective to the whole research. A compilation of the responses is given in Table 7.1. Following section gives a summary of the responses to the questions.

7.3 Responses from Industries to the Questionnaire

The responses from the industrialists to the questionnaire have been summarized and given below. A compilation of individual responses are given in Table 7.1.

1) Does your company do methodical evaluations of process designs for operability/controllability to guide process design at the PFD stage?

There were as many positive responses as negative to this question.

2) If Yes, what are the criteria that you evaluate it upon, and what methods do you use to analyze the criteria?

Some of the criteria that the industries stressed upon and which have already been

Table 7. 1Compilation of Comments from Industry

#	Company	1	2	3	4	5
1	Brown & Root, Inc.	NO	N/A	More money in little time	EF, Availability	
2	Celanese	YES	At start up; Product quality	N/A	Specified product quality, But lower rate; same quality and rate; specified rate and lower quality.	Illustrate the three criterion in 4 with non-classified PFDs from industries.
3	Eastman Chemical Co.	YES	No rigorous operability study; Sensitivity of unit and control strategy with respect to controllability	N/A	Profitability; Steady-State disturbance analysis, dynamic Behavior as a function of holdup.	Tool based on steady state with dynamic information like holdup. Identify hidden problems; Easy to use screening tool
4	Eastman Kodak Co.	NO	N/A	Photographic films company; O perability not very important	Good dynamics No noise; Operability with constraints	Easily applicable and understandable
*5	Elf Atochem	Y for Aspen runs	In Aspen runs, product quality and profitability	Time rush; No available method to do the study	Quality, possible location of key control parameters, cost/profit	Simple to use tool and easily 'linkable' to Aspen like software
6	Exxon	YES	Safety and Operability; side reactions; avoid re-work after installation	N/A	Safety, health, Environmental Impact and human factors or ergonomics	None as they do it. Chemical Engineers learn PFDs, P&IDs and OSHA guidelines.
*7	Gensym	YES	Controllability, data validity, soft sensor predictability.	N/A	Profitability, dependability and quality	Show financial benefits and give information on others successes
*8	Goodyear Tire & Rubber Company	NO	N/A	Operability study done at P&ID stage	Controllability, safety, product quality, environmental impact	Simple to use, show increase in benefits.

* Member/participant of Measurement and Control Engineering Center.

1. Does your company do methodical evaluations of process designs for operability/controllability to guide process design at the PFD stage?
2. If Yes, what are the criteria that you evaluate it upon, and what methods do you use to analyze the criteria?
3. If No, why don't you think it is necessary to evaluate the designs based on these criteria?
4. What criteria for operability/controllability do you think should be looked into to evaluate a process design?
5. What should academia do to provide you with an incentive to perform the operability/controllability analysis and evaluate process designs?

*9	Industrial Systems Design	2,3,4 N/A as work involves building and selling control programs, no process designing. 5) Start with contacting mid-sized companies as they are unaware of work of this kind				
10	Kimberly-Clark	NO	N/A	Not part of project cycle of paper industry	Intrinsic stability; Safety; meet design requirements	Profitability; improve operating efficiency.
*11	Lubrizol Corp.	YES	Process Hazards Analysis, HAZOP	P&ID are needed for any detailed analysis	Vessel residence times, environmental impact and waste minimization	Better engineering tools
12	Lyondell-Citgo	NO	N/A	Should be done in HAZOP stage with P&IDs	Safety, Reliability, good control strategies	Dynamic simulation as a tool; Steady State simulation for specifying control points
13	Mobil Tech.	NO	N/A	Operability very challenging; more stress on economics;	Location of instrumentation; From 3 economics too.	Will reply later
14	M. W. Kellogg	YES	Tools in CONSYD or own criteria	N/A	Integral Control; process Interactions; surge capacities	Develop tools; Provide case studies and ex.
15	Olin Chemicals	YES	Pilot plant to test for Operability, or a Thermdynamic model like Aspen. No PFD.	N/A	Happy with Aspen Plus (talking about methods and not criteria)	Work on physical properties for simple model databanks
16	Pharmacia & Upjohn	YES	Controllability, piping, Enviromental operational hazards	N/A	Profitability, quality, Safety, Environmental Impact, laws	Improvement beyond their current approach
17	Phillips Petroleum	NO	N/A	P&ID required for Operability study	Dynamic model	
18	Phillips Petroleum	Yes for reactor NO for rest.	Heat management, for reactor important at design for temperature control.	Mechanical design. & dynamic model required for Operability study.	Equipment response to upsets, feed composition & rate, control, overdesign, Min & max Temps.	Economical; easy for design engineer; should be solution to problem overlooked by company till then.

* Member/participant of Measurement and Control Engineering Center.

1. Does your company do methodical evaluations of process designs for operability/controllability to guide process design at the PFD stage?
2. If Yes, what are the criteria that you evaluate it upon, and what methods do you use to analyze the criteria?
3. If No, why don't you think it is necessary to evaluate the designs based on these criteria?
4. What criteria for operability/controllability do you think should be looked into to evaluate a process design?
5. What should academia do to provide you with an incentive to perform the operability/controllability analysis and evaluate process designs?

19	Praxair	Y for new design; No for standard	Steady state Controllability (RGA); Dynamic simulation for designing alternatives.	Past experience sufficient	Profitability; Simple metrics of Controllability/Operability	Show profitability; simple for any Process. Engineer; Integrated into standard. simulation. Package like Aspen, Hysys
*20	Union Carbide Corp.	Y if required; N for proven designs	Controllability with best control design; Operability During start up and after severe disturbances; validation of product quality control	For proven designs, operability study does not give any additional benefits	Stable, self-regulating; prefer process operating safely and stably with controllers out-of-service to one requiring all instrumentation to be in top shape in order to operate.	Develop tools that simplify process modeling and easy to use; Should produce quick result; Should be compatible with the ASPEN suite.
*21	Velsicol Chemical Corporation	No	N/A	Limited resources and a general lack of in-house expertise, but is a valuable study.	early evaluation of measurement technology requirements; Control schemes should be robust and workable (avoid loop interactions, split-range controls, etc.).	Provide study data that quantifies the value of early process control/operability reviews. Develop tools and methodologies that facilitate these design evaluation efforts.

* Member/participant of Measurement and Control Engineering Center.

1. Does your company do methodical evaluations of process designs for operability/controllability to guide process design at the PFD stage?
2. If Yes, what are the criteria that you evaluate it upon, and what methods do you use to analyze the criteria?
3. If No, why don't you think it is necessary to evaluate the designs based on these criteria?
4. What criteria for operability/controllability do you think should be looked into to evaluate a process design?
5. What should academia do to provide you with an incentive to perform the operability/controllability analysis and evaluate process designs?

studied by this research are controllability, safety, environmental impact and profitability. There are some additional criteria that have been suggested by industries and these are product quality, sensitivity of units to disturbances (which again is a measure of the controllability of the unit and the process), HAZOP studies, data validity and soft sensor predictability. They would also like to avoid dangerous side reactions and any additional work after installation as much as possible. Some of the tools that they have adopted for the operability studies are CONSYD, pilot plants thermodynamic models in ASPEN, and dynamic simulation to design alternatives.

3) If No, why don't you think it is necessary to evaluate the designs based on these criteria?

This is the most interesting part of the questionnaire for the current research as the responses to this question answered the query as to why industries do not indulge in operability studies, which appears from an academic point of view, to be the most crucial step in industry. The most common response was that operability study can not be done at the process flow diagram (PFD) stage. A process and instrumentation diagram (P&ID) is very essential to perform operability analysis of the process. Some industries, like the paper and photographic films responded that operability studies are not a part of their project cycle and they work only on those factors that contributed towards the enhancement of their product. Some were satisfied with their designs based on past experience, and consider it uneconomical to spend so much time and effort on an operability analysis. A personal communication with one of the industrialists gave to understand that most of the times industry would expend its resources on only those conditions required to operate the process that prove to be lucrative in both money and time.

4) What criteria for operability/controllability do you think should be looked into to evaluate a process design?

   The responses to this question were very informative as, they were given by people based on their vast experience in industry. The responses were drawn from different fields and many past experiences. One of the most important criteria that they deemed was important for the process to be considered operable was again profitability. Other criteria that have already been touched upon were environmental impact, product quality, controllability, good dynamics and the process should meet design requirements. Some new factors like health and human factors or ergonomics, intrinsic stability, instrumentation location, reliability, noiselessness, equipment response to upsets and vessel residence times and availability have also been added.

5) What should academia do to provide you with an incentive to perform the operability/controllability analysis and evaluate process designs?

   The responses to this question give academia a sharper focus in this field. The major demand from the industries to the academia is that they design a tool for the operability studies that is easy to apply and can be used by any process engineer and not by someone proficient in advanced process control alone. Again, the importance of profitability has been stressed. Chemical engineers should get more familiar with P&IDs and OSHA guidelines. A tool based on both steady state information, for specifying control points, and dynamic information should be developed. Also, the tool should be compatible to standard simulation packages like ASPEN PLUS™ and HYSYS.

7.4 Summary

In summary the most common responses were that the companies want to make as much profit in as little time as possible. They would subject their processes to an operability study only under the conditions that the tool for that purpose is simple to use and is proven to increase the profitability of their operations.

From the survey on industries, it can be concluded that the current research is valuable, as confirmed by the industrialists. The operability criteria that they suggested matched well with the criteria that this research started with, and added more to the criteria list too (See Table 8.1). This proves that the current research is very valuable in improving the operability and feasibility of industrial processes. The task ahead is to convince industries to accept this work and implement operability studies in industries too. This can be done with a frequent exchange of information between industries and academia, which Hashimoto (1995) said there was an immediate need for, and later Schijndel (1999) showed that the gap between academia and industry has been substantially bridged. The conclusions from this work and future directions are discussed in more detail in Chapter 9.

Chapter 8

RESULTS

8.1 Results

This research work resulted in the development of a framework to build a foolproof method to perform feasibility and operability analysis on industrial processes and evaluate for their acceptability in industry. Simple tools have been proposed to evaluate process designs for their profitability, environmental impact and controllability. These tools have been coded in ASPEN PLUS™ 's user unit operation model. The final result is that a user model with tools to evaluate controllability (C), profitability ($) and environmental impact (E) has been developed. Thus, this model can be used as a template and any design can be run with it, except for the few changes that need to be made to suit that particular chemical process.

Two case studies, hot and cold water mixing system and manufacture of methyl chloride by hydrochlorination of methanol have been used to test the tools and the code developed for C, $ and E analyses. The significance of the interaction between design and control has also been discussed. The hot and cold water system has been used for controllability analysis alone, while the methyl chloride process has been used for all three analyses.

A comparison of three alternate designs for the methyl chloride process has been done with two control strategies. The results for the comparison using Strategy 1 (where product flowrate (*PROD; CV1*) is controlled by feed flowrate (*FEED; MV1*), and product purity (*XPRD; CV_2*) is controlled by heat supply to feed preheater, (*HEATH; MV2*)) are shown in Table 8.1.

Table 8. 1 Comparing Alternate Designs of the Methyl Chloride Process with Control Strategy 1

	Adiabatic PFR (Alternate 1)	Isothermal PFR (Alternate 2)	CSTR (Alternate 3)
Controllability (CN)	25.4	36.0	23.7
Environmental Impact (EIU/kg)	287.5	207.8	303.5
Profitability ($/yr)	2.48M	6.39M	1.73M

The profits obtained (2.48 M$/yr) for Alternate 1 in this research vary slightly from the profit obtained (2.2 M$/yr) in Dantus's research (1999), from which, Alternate 1 has been chosen as the initial steady state optimum system for this research. The difference in the results is because Dantus included liability, fine and penalties charges in his economic analysis. These are ignored in the current research as they do not add up to a significant figure, and also the economic analysis in this research was focussed more on an overall analysis rather than on environmental economics.

The results in Table 8.1 show that Alternate 3 is most controllable, but has maximum environmental impact and least profits. Alternate 2 has least environmental impact and generates maximum profits, but is most uncontrollable (highest CN). These results show the competing nature of these criteria. Thus, to make a decision based on all these competing criteria together, an overall index is required. This index is proposed in the next section. Similar trends were also observed for control strategy 2 (See Chapter 6).

Another major phase of this work is that a questionnaire has been sent to 75 industries regarding operability analysis in their area. The industrial survey has given a very valuable insight into the actual operations of the industrial processes. The responses from them have been compiled and utilized to expand the scope of future work (See Chapter 7). The industrial survey has also helped in expanding the list of criteria that this work originally started with and are given in Table 8.2.

The main objectives of this work were to show all the factors that go into making a chemical process acceptable in industry and, also compare alternatives with respect to these factors. The factors that this work started with (See Section 3.1.2), fortified by the responses from industry resulted in an expanded list of criteria as shown in Table 8.2.

Table 8. 2 Expanded List of Criteria for Feasibility and Operability Studies

Initial Criteria	Industrial Input
Profitability	Product Quality
Environment friendly	Ergonomics
Controllability	Intrinsic stability
Resiliency	Instrumentation Location
Flexibility	Reliability
Safety	Noiselessness
	Availability

Since experienced industrialists have themselves stated that these conditions and criteria are important for a process to be feasible and acceptable in industry, the first objective has been achieved. The case studies (See Chapters 5 and 6) and the simple tools developed and tested on the cases have helped in accomplishing the second objective and also showed that any process can be evaluated based on all these conditions by a simple methodology (See Chapter 3).

8.2 Principal Result

The major achievement of this work is that a simple methodology has been proposed for feasibility and operability analysis. The objective of the current work and the future work is to develop a simple methodology to evaluate a process design for its ability to operate in a manner that satisfies the gamut of F&O criteria that have already been discussed in previous sections/chapters. Based on this objective, the methodology proposed is that when sufficient number of criteria have been gathered and simple tools have been developed to measure them quantitatively, based on the index values of each of the criteria, either by AHP or multi-objective optimization (MOO), an overall F&O index should be calculated. This F&O index should be used to compare alternative process designs.

The methodology is better illustrated in Table 8. 3. The table lists all the criteria for operability gathered so far along with the feasibility criteria, and shows three alternate designs, A, B and C. The proposed methodology says that Table 8.3 should be filled and then finally the last row, i.e., the values of the F&O index should be calculated for all designs. The F&O index alone should be good enough to compare alternate designs and propose the best acceptable design for implementation in industry. Filling up Table 8.3,

Table 8. 3 Proposed Methodology for Operability Analysis

S.No.	Criterion	Design A (Alternate 1)	Design B (Alternate 2)	Design C (Alternate 3)
1	Profitability ($/yr)			
2	Environmental Impact (EIU/kg)			
3	Controllability			
4	Resiliency			
5	Flexibility			
6	Safety			
7	Product Quality			
8	Stability			
9	Reliability			
10	Noiselessness			
11	Availability			
12	**Feasibility & Operability**			

developing an overall F&O index to compare alternative process designs and, offering the work to industries is the goal that academia should strive to achieve. A summary of the major contributions and results of this research is given in the next section.

8.3 Major Contributions of this Research

1) Developed a methodology to perform operability analysis in the design phase.
2) Coded the tools to evaluate profitability, environmental impact and controllability in ASPEN PLUS™.
3) Proposed a systematic procedure to quantitatively select among alternatives when issues such as controllability, economics and environmental impact are considered.
4) Two cases have been used to apply and test the developed methods.
5) A survey on operability analyses in industries has been done and the input from industries is utilized to expand the course of future work.
6) An ultimate goal is proposed which considers the development of an overall feasibility and operability index.

These results lead to some significant conclusions, which are discussed in the next chapter (Chapter 9).

Chapter 9

CONCLUSIONS AND FUTURE RECOMMENDATIONS

9.1 Conclusions

The most important conclusion from this research comparing alternatives based on feasibility and operability criteria is work is a simple task. Also, a systematic feasibility and operability study should be adopted in every industry at the design stage regardless of whether the process has been tested for its feasibility, which is the profitability and environmental friendliness of the process. Unfortunately the truth is that there are very few industries that go through the steps of conducting an operability study and concentrate on the feasibility of the process. This work started with some criteria for operability. The input from industries has expanded the list, which shows that the list of criteria for operability can never be exhaustive. The intricacies of the chemical processes and the variations from one process to another add more criteria to the list. From previous chapters, the conclusion that can be drawn is that all the criteria are equally important.

Overlooking any feasibility or operability criteria will ultimately bring losses to the industry. A very common observation from the industrial survey is that industry is mainly concerned about the time and money involved in any project. As has been stated at the beginning of this section not many industries undertake operability studies to evaluate their processes. They more often base their designs on past experiences as they believe that, that will save them a lot of time as well as money. But, the simple tools developed in this work to evaluate a few criteria rule out the time factor.

The most common response to the question as to what academia should do to provide industries with an incentive to accept their research work is that the tool developed by the academia for feasibility and operability studies should be easy to use for any process engineer and the tool should prove that the profitability of the company would be enhanced if it is used for the F&O studies. This response gives a strong motivation for this work to be followed up, the reasons being that:

- The tools that were used to evaluate the alternative designs of the case studies for operability criteria has proved that simple tools can be used to conduct operability studies.
- With the profitability study, alternate designs can be easily compared and the best design selected based on their profitability, which is what the industries are most interested in.
- Finally, the coding done for this part of the work in Aspen Plus™ has been very simple and made very user friendly. The code does not demand much work or time from the user to utilize its benefits.

The aforesaid reasons are motivating enough to continue this work on the same lines. From a practical view, any work done by the academia should be acceptable to industry as otherwise, the purpose of the work is defeated. The input from industry showed that they realize the value of this kind of operability study with which they can easily compare alternative designs to their processes and select the best. But they do not accept the study because of practical limitations like not being able to find a simple and practical tool. Thus, since this work proved to be valuable and acceptable to industry, the immediate focus should be to collaborate more with industries and develop a tool that meets with the industrial requirements. Based on these conclusions, some recommendations for future work have been made, and these are given in the next section.

9.2 Future Recommendations

- Establish more contacts with industries and obtain as much input as possible from them to sharpen the focus of future work.
- Prove the value of operability study to industry by conducting a three design example: 1) Design 1: Without feasibility or operability analyses. 2) Design 2: With feasibility and without operability analyses. 3) Design 3: With both feasibility and operability analyses. As has been demonstrated with the methyl chloride process (See Table 6.9), these three designs would prove that the economics of the designs would improve from design 1 to design 3 over a period of time. In essence, this example would prove that the economics would improve when both feasibility and operability studies are included as opposed to conducting none or feasibility study alone.
- Find more criteria to add to the expanded list of criteria given in Chapter 8 (See Table 8.2).
- Develop quantitative measures for the criteria in the expanded list of criteria that haven't been worked upon in this work, to help perform a more rigorous comparison of alternatives.

- An alternate tool needs to be found for controllability analysis, based on the discussion in Chapter 4.
- Explore the possibility of using Analytic Hierarchy Process or Multiple Objective Optimization (See Appendix F) for operability studies.
- Find other software tools, which are more suitable for the analysis of all criteria.
- Incorporate all tools into one complete package of Aspen or any other software found suitable for the work.
- Make the package as user friendly and as simple to use as possible.

The final result is a simple tool for industry to use.

BIBLIOGRAPHY

Alva-Argaez, A., A. C. Kokossis and R. Smith (1998). "Wastewater Minimization of Industrial Systems Using an Integrated Approach." Computers and Chemical Engineering **22**(Supplement): S741-S744.

Ammann, P. R., G. S. Koch, M. Alexis Maniatis (1995). "It Makes More Sense to be Proactive than Reactive: The Best Approach to Environmental Compliance." Chemical Engineering **102**(2): 104-110.

Arkun, Y. (1986). Dynamic Process Operability: Important Problems, Recent Results and New Challenges. International Conference on Chemical Process Control-3rd, Asilomar, California.

Aspen Technology, Inc. (1995). "User Models." ASPEN PLUS^{TM} Reference Manual 6(5): 1-10.

Auguston, K. (1995). "Cost Justification: More Than a Numbers Game." Modern Materials Handling 1995(September): 37-39.

Bahri, P. A., J. A. Bandoni, and J. A. Romagnoli (1997). "Integrated Flexibility and Controllability Analysis in Design of Chemical Processes." AIChE Journal **43**(4): 997-1015.

Balling, R. (1999). City Planning Via a MultiObjective Genetic Algorithm and a Pareto Set Scanner. Optimization in Industry - II, Banff, Alberta, Canada, ASME.

Barton, G. W., W. K. Chan, J. D. Perkins, and R. G. H. Prince (1986). "Controllability Analysis of Alternative Process Designs". CHEMECA 86, Adelaide.

Beaves, R. G. (1993). "The Case for a Generalized Net Present Value Formula." The Enginering Economist **38**(2): 119-133.

Belanger, P. W. and W. L. Luyben (1998a). "Plantwide Design and Control of Processes with Inerts. 1. Light Inerts" Industrial Engineering Chemistry and Research **37**(2): 516-527.

Belanger, P. W. and W. L. Luyben (1998b). "Plantwide Design and Control of Processes with Inerts. 2. Heavy Inerts." Industrial Engineering Chemistry and Research **37**(2): 528-534.

Belanger, P. W. and W. L. Luyben (1998c). "Plantwide Design and Control of Processes with Inerts. 3.Intermediate Inerts." Industrial Engineering Chemistry and Research **37**(2): 535-546.

Bouwes, N. W. and S. M. Hassur (1997a). Toxic Release Inventory Relative Risk-Based Environmental Indicators Methodology. Washington DC, United States Environmental Protection Agency.

Bouwes, N. W. and S. M. Hassur (1997b). Toxic Release Inventory Relative Risk-Based Environmental Indicators: Interim Toxic Weighting Summary Document. Washington DC, United States Environmental Protection Agency.

Bristol, E. H. (1966). "On a New Measure of Interaction for Multi-Variable Process Control." IEEE Transactions on Automatic Control **11**(1): 133-134.

Bryson, N. and A. Mobolurin (1994). "An Approach to Using the Analytic Hierarchy Process for Solving Multiple Criteria Decision Making Problems" European Journal of Operational Research **76**: 440-434.

Canada, J. R., W. G. Sullivan, and J. A. White (1996). Capital Investment Analysis for Engineering and Management. New Jersey: Prentice Hall, Inc.

Carr, C. and C. Tomkins (1996). "Strategic Investment Decisions: The Importance of SCM. A Comparitive Analysis of 51 Case Studies in U.K., U.S. and German Companies." Management Accounting Research **7**: 199-217.

Chacon-Mondragon, O. L. and D. M. Himmelblau (1996). "Integration of Flexibility and Control in Process Design." Computers and Chemical Engineering **20**(4): 447-452.

Ciric, A. R. and S. G. Huchette (1993). "Multiobjective Optimization Approach to Sensitivity Analysis: Waste Treatment Cost in Discrete Process Synthesis and Optimization Problems." Industrial and Engineering Chemistry Research **32**: 2636-2646.

Clark, P. A. and A. W. Westerberg (1983). "Optimization for Design Problems Having More Than One Objective." Computers and Chemical Engineering **7**: 259-276.

CMR (1997). "Chemical Profile: Methyl Chloride." Chemical Marketing Reporter **1997**(November): 37.

CMR (1999). "Chemical Prices." Chemical Market Reporter **255**(18): 22-29.

Dantus, M. M. (1995). "Waste Minimization and Process Integration Applied to the Retrofit Design of Chemical Processes." MS Thesis, Oklahoma State University.

Dantus, M. M. L. (1999). "Methodology for the Design of Economical and Environmentally Friendly Processes: An Uncertainty Approach." Ph.D. Dissertation, Oklahoma State University.

Davis, G. A., L. Kincaid, M. Swanson, T. Schultz, J. Bartmess, B. Griffith, and S. Jones (1994). Chemical Hazard Evaluation for Management Strategies: A Method for Ranking and Scoring Chemicals by Potential Human Health and Environmental Impacts. US Environmental Protection Agency, EPA/600/R-94/177.

Douglas, J. M. (1985). "A Hierarchical Decision Procedure for Process Synthesis." AIChE Journal **31**(3): 353-362.

Douglas, J. M. (1992). "Process Synthesis for Waste Minimization." Industrial and Engineering Chemistry Research **31**(1): 238-243.

Downs, J. J., A. C. Hiester, S. M. Miller and K. B. Yount (1994). "Industrial Viewpoint on Design/Control Tradeoffs." IFAC Integration of Process Design and Control, ed. E. Zafiriou.

Downs, J. J. and B. Ogunnaike (1995). Design for Control and Operability: An Industrial Perspective. Foundations of Computer Aided Process Design, Snowmass, CO, CACHE, AIChE.

Dyer, J. A. and K. L. Mulholland (1998). "Prevent Pollution via Better Reactor Design and Operation." Chemical Engineering Progress **94**(2): 61-66.

Eliceche, A. M., M. Sanchez and L. Fernandez (1998). "Feasible Operating Region of Natural Gas Plants Under Feed Perturbations." Computers and chemical engineering **22**(Supplement): S879-S882.

Fisher, W. R., M. F. Doherty, and J. M. Douglas (1984). "Synthesis of Steady State Control Structures for Complete Chemical Plants. Part 3: Control Structure Synthesis Strategies." AIChE, Winter National Meeting, New York.

Fisher, W. R., M. F. Doherty, and J. M. Douglas (1985a). "Evaluating Significant Economic Trade-Offs for Process Design and Steady-State Control Optimization Problems." AIChE **31**(9): 1538-1547.

Fisher, W. R., M. F. Doherty, and J. M. Douglas. (1985b). "Steady State Control as a Prelude to Dynamic Control." Chemical Engineering Research and Design **63**: 353-357.

Fisher, W. R., M. F. Doherty, and J. M. Douglas (1988a). "The Interface Between Design and Control. 1.Process Controllability." Industrial and Engineering Chemistry Research **27**(4): 597-605.

Fisher, W. R., M. F. Doherty, and J. M. Douglas (1988b). "The Interface Between Design and Control. 2.Process Operability." Industrial and Engineering Chemistry Research **27**(4): 606-611.

Fisher, W. R., M. F. Doherty, and J. M. Douglas (1988c). "The Interface Between Design and Control. 3. Selecting a Set of Controlled Variables." Industrial and Engineering Chemistry Research **27**(4): 611-615.

Gowland, R. (1996). "Putting Numbers on Inherent Safety." Chemical Engineering **103**(3): 82-86.

Goyal, R. K. (1993). "Hazops in Industry." American Society of Safety Engineers **38**(8): 34-.

Grossmann, I. E. and K. P. Halemane (1982). "Decomposition Strategy for Designing Flexible Chemical Plants." AIChE Journal **28**(4): 686-696.

Grossmann, I. E. and M. Morari (1983a). "Operability, Resiliency and Flexibility-Process Design Objectives for a Changing World". Foundations of Computer-Aided Process Design: Second International Conference, Snowmass, Colorado, CACHE.

Grossmann, I. E., K. P. Halemane and R. E. Swaney (1983b). "Optimization Strategies for Flexible Chemical Processes." Computers and Chemical Engineering **7**(4): 439-462.
Hashimoto, I. and E. Zafiriou (1995). Design for Operations and Control. Foundations of Computer-Aided Process Design, Snowmass, CO.

Harris, T. J. (1993). Quality Issues in Process Design and Process Operations. Foundations of Computer Aided Process Operations, Crested Butte, CO, CACHE and CAST Division of AIChE.

Hashimoto, I. and E. Zafiriou (1995). Design for Operations and Control. Foundations of Computer-Aided Process Design, Snowmass, CO.

Holt, R. B. and M. Morari (1985). "Design of Resilient Processing Plants-6. The Effect of Right-Half-Plane Zeros on Dynamic Resilience." Chemical Engineering Science **40**(1): 59-74.

Huang, Y. L. and L. T. Fan (1992). "Distributed Strategy for Integration of Process Design and Control: A Knowledge Engineering Approach to the Incorporation of Controllability into Exchanger Network Synthesis." Computers and Chemical Engineering **16**(5): 497-522.

Johnston, R. D. and G. W. Barton Control System Development without Dynamic Simulation.

Johnston, R. D. and G. W. Barton (1987). "Design and Performance Assessment of Control Systems using Singular Value Analysis." Industrial Engineering Chemistry and Research **26**(4): 830-839.

Klema, V. C. and A. J. Laub (1980). "The Singular Value Decomposition: Its Computation and Some Applications." IEEE Transactions on Automatic Control **AC-25**(2): 164-176.

Lenhoff, A. M. and M. Morari (1982). "Design of Resilient Processing Plants-1: Process Design Under Consideration of Dynamic Aspects." Chemical Engineering Science **37**(2): 245-258.

Lewin, D. R. (1996). "A Simple Tool for Disturbance Resiliency Diagnosis and Feedforward Control Design." Computers and Chemical Engineering **20**(1): 13-25.

Linnhoff, B. and E. Kotjabasakis (1986). "Process Optimization: Downstream path for Operable Process Design." Chemical Engineering Progress **1986**(May): 23-28.

Luyben, W. L. and M. L. Luyben (1997). Essentials of Process Control, The McGraw-Hill Companies, Inc.

Mallick, S. K., H. Cabezas, C. J. Bare and K. S. Sikdar (1996). "A Pollution Reduction Methodology for Chemical Process Simulators." Industrial Engineering Chemistry Research **35**(11): 4128-4138.

Manousiouthakis, V. and D. Allen (1995). "Process Synthesis for Waste Minimization." Foundations of Computer Aided Process Design, Snowmass, CO, CACHE (Computer Aids for Chemical Engineering Education).

Mansfield, D. P. (1996). "Viewpoints on Implementing Inherent Safety." Chemical Engineering **103**(3): 78-80.

Marselle, D. F., M. Morari, and D.F. Rudd (1982). "Design of Resilient Processing Plants-2: Design and Control of Energy Management Systems." Chemical Engineering Science **37**(2): 259-270.

McAvoy, T. J. (1987). Integration of Process Design and Process Control. Recent Developments in Chemical Process and Plant Design, ed. Y. A. Liu and H. McGee Jr., A., John Wiley & Sons: 289-324.

Milbourn, T. T. (1996). "The Executive Compensation Puzzle: Theory and Evidence." IFA Working Paper **235,** London Business School.

Moore, C. (1986). "Application of Singular Value Decomposition to the Design, Analysis and Control of Industrial Processes". American Control Conference.

Morari, M. (1983a). "Design of Resilient Processing Plants-3." Chemical Engineering Science **38**(11): 1881-1891.

Morari, M. (1983b). "Flexibility and Resiliency of Process Systems." Computers and Chemical Engineering **7**(4): 423-437.

Morari, M. and J. Perkins (1995). "Design for Operations". Fourth International Conference on Foundations of Computer-Aided Process Design, Snowmass, CO, CACHE, American Institute of Chemical Engineers.

Naot, I. and D. R. Lewin (1995). "Analysis of Process Dynamics using Steady State Flowsheeting Tools. Dynamics and Control of Chemical Reactors, Distillation Columns and Batch Processes". DYCORD+, '95, Copenhagen, Denmark.

Narraway, L. T. and J. D. Perkins (1993). "Selection of Process Control Structure Based on Linear Dynamic Economics." Industrial Engineering Chemistry & Research **32**(11): 2681-2692.

Narraway, L. T., J. D. Perkins, and G. W. Barton (1991). "Interaction Between Process Design and Process Control: Economic Analysis of Process Dynamics." Journal of Process Control **1**(5): 243-250.

Ogunnaike, B. A. and H. W. Ray (1994). Process Dynamics, Modeling and Control. New York: Oxford University Press.

Ostrovsky, G. M., Y. M. Volin and D. V. Golovashkin (1996). "Evaluation of Chemical Processes Flexibility." Computers and Chemical Engineering **20**(Supplement): S617-S622.

Palazoglu, A. and Y. Arkun (1986). "A MultiObjective Approach to Design Chemical Plants With Robust Dynamic Operability Characteristics." Computers and Chemical Engineering **10**(6): 567-575.

Palazoglu, A. and Y. Arkun (1987). "Design of Chemical Plants with Multi Regime Capabilities and Robust Dynamic Operability Characteristics." Computers and Chemical Engineering **11**(3): 205-216.

Palazoglu, A., B. Manousiouthakis and Y. Arkun (1985a). "Design of Chemical Plants with Improved Dynamic Operability in an Environment of Uncertainty." Industrial Engineering and Chemical Process Design and Development **24**(3): 802-813.

Perkins, J. D. and M. P. F. Wong (1985b). "Assessing Controllability of Chemical Plants." Chemical Engineering Research And Design: Transactions of the Institution of Chemical Engineers **63**(November): 358-362.

Peters, M. S. and K. D. Timmerhaus (1991). Plant Design and Economics for Chemical Engineers. New York, McGraw-Hill.

Press, W. H., S. A. Teukolsky, W. T. Vetterling, Flannery, and Brian P. (1992). Numerical Recipes in Fortran: The Art of Scientific Computing. New York, Press Syndicate of the University of Cambridge.

Pumps, B. (1996). "Integrating Process Design and Control Improves Plant Operability." Oil and Gas Journal **1996**(July): 67-69.

Ramchandran, S. (1998). "Consider Steady State Models for Process Control". Chemical Engineering Progress **94**(2): 75-81.

Rovaglio, M., T. Faravelli, P. D. Gaffuri, DiPalo, C and. Dorigo, A.. (1995). "Controllability and Operability of Azeotropic Heterogeneous Distillation Systems." Computers and Chemical Engineering **19**(Supplement): S525-S530.

Saaty, T. L. (1994). "How to Make a Decision: The Analytic Hierarchy Process." Interfaces **24**(6): 19-43.

Saaty, T. and E. Forman (1999). "Click Here for Decisions." Expert choice, Inc.

Saboo, A. K. and M. Morari (1984). "Design of Resilient Processing Plants-8: A Resilience index for heat exchanger networks." Chemical Engineering Science **40**(8): 1553-1565.

Schijndel, J. V. and E. N. Pistikopoulos (1999). Towards the Integration of Process Design, Process Control and Process Operability - Current Status and Future Trends. FOCAPD'99, Breckenridge, CO.

Seborg, D. E., T. F. Edgar, and D. A. Mellichamp (1989). Process Dynamics and Control, John Wiley & Sons.

Seferlis, P. and J. Grievink (1999). Plant Design based on Economic and Static Controllability Criteria. FOCAPD'99, Breckenridge, CO.

Shank, J. K. (1996). "Analyzing Technology Investments-from NPV to Strategic Cost Management (SCM)." Management Accounting Research **7**: 185-197.

Shimizu, K. and M. Matsubara (1985). "Directions of Disturbances and Modeling Errors on the Control Quality in Distillation Systems." Chemical Engineering Communications **37**: 67-91.

Shinskey, F. G. (1983). "Uncontrollable Processes and What to Do About Them." Hydrocarbon Processing 1983(November): 179-182.

Stermole, F. J. and J. M. Stermole (1996). Economic Evaluation and Investment Decision Methods. Golden, Co, Investment Evaluations Corporation.

Stewart, G. B. I. (1991). The Quest for Value. New York, Harper Business.

Straub, D. A. and I. E. Grossmann (1990). "Integrated Stochastic Metric of Flexibility for Systems with Discrete State and Continuous Parameter Uncertainties." Computers and Chemical Engineering **14**(9): 967-985.

Swaney, R. E. and I. E. Grossmann (1985a). "An Index for Operational Flexibility in Chemical Process Design. Part 1: Formulation and Theory." AIChE Journal **31**(4): 621-630.

Swaney, R. E. and I. E. Grossmann (1985b). "An Index for Operational Flexibility in Chemical Process Design. Part 2: Computational Algorithms." AIChE Journal **31**(4): 631-641.

Terrill, D. L. and J. M. Douglas (1987a). "Heat-Exchanger Network Analysis. 1. Optimization." Industrial and Engineering Chemistry Research **26**(4): 685-691.

Terrill, D. L. and J. M. Douglas (1987b). "Heat Exchanger Network Analysis. 2. Steady-State Operability Evaluation." Industrial and Engineering Chemistry Research **26**(4): 691-696.

Thomaidis, T. V. and E. N. Pistikopoulos (1994). "Integration of Flexibility, Reliability and Maintenance in Process Synthesis and Design." Computers and Chemical Engineering **18**(Supplement): S259-S263.

Turton, R., R. C. Bailie, W.B. Whiting, and S. A. Joseph (1998). Analysis, Synthesis and Design of Chemical Processes. New Jersey: Prentice Hall, PTR.

Tyreus, B. D. and M. L. Luyben (1999). Industrial Plantwide Design for Dynamic Operability. FOCAPD'99, Breckenridge, CO.

van der Helm, D. U. (1997). An Economic Case Study of Process Modification for the Allyl Chloride Process. MS Thesis. Stillwater, Oklahoma State University: 111.

Vijuk, R. and H. Bruschi (1988). "AP600 Offers a Simpler Way to Greater Safety, Operability and Maintainability." Nuclear Engineering International 1988(November): 22-26.

Webb, C. M. and M. A. Waronker (1993). "DCS Installation gives Plantwide Process Control." Water/ Engineering & Management 1993(August): 27-29.

Weitz, O. and D. R. Lewin (1996). "Dynamic Controllability and Resiliency Diagnosis Using Steady State Process FLowsheet Data." Computers and Chemical Engineering **20**(4): 325-335.

Wentworth, C. E. and T. H. Russell (1993). "Guidelines Useful for Incorporating DCS in Existing Process Plant." Oil and Gas Journal 1993(Nov 29): 74-78.

White, J. A., K. E. Case, and B. P. Dravid (1998). Principles of Engineering Economic Analysis. New York: John Wiley & Sons, Inc.

Yi, C. K. and W. L. Luyben (1995). "Evaluation of Plant-Wide Control Structures by Steady-State Disturbance Sensitivity Analysis." Industrial Engineering Chemistry and Research **34**(7): 2393-2405.

Ziegler, J. G. and J. R. Connell (1994a). "For Optimum Control: Modify the Process and Not the Controls." Chemical Engineering **101**(5): 132-140.

Ziegler, J. G. and J. R. Connell (1994b). "For Optimum Control: Modify your Process. Part 2." Chemical Engineering **101**(7): 107-116.

Ziegler, J. G., N. B. Nichols, and N. Y. Rochester (1943). "Process Lags in Automatic-Control Circuits." Transactions of the ASME **65**: 433-444.

APPENDIX A

METHODOLOGY

This chapter gives a stepwise procedure to perform a quantitative analysis of feasibility and operability and use the code programmed in Aspen for F&O analysis to evaluate a chemical process for its controllability, environmental impact and profitability. The result of following these steps would be to obtain the values of the indices of the three criteria mentioned above for a process and its alternatives, and thus help in comparing them. Based on the best values of the indices, the best design can be proposed. Figures A.5, A.6, A.7 and A.8 give these steps in the form of a flowsheet for overall feasibility and operability or individual controllability, environmental impact and profitability.

A.1 Steps to Follow

1. The chemical process to be studied should be first simulated in Aspen Plus™ by creating its flowsheet in Aspen's model manager, inputting the data required for the process to work and then running it.
2. The USER2 model is selected for coding the singular value analysis. Following is a description of the USER models in ASPEN PLUS™.

The USER models in ASPEN PLUS™ consist of one or more Fortran subroutines that are written by the user when the models provided by Aspen do not meet with the needs of the user. There are six kinds of user models, one of which is the user unit operation model. The user unit operation model allows the user to interface his own unit operation model with ASPEN PLUS™ by supplying a subroutine and entering the name of the routine in the input file (Aspen Technology, 1995). There are two types of unit operation models: USER and USER2. One of these two should be selected for developing the F&O analysis tool. While USER allows only four inlet and four outlet streams, USER2 has no limit on the number of inlet or outlet streams. Since an industrial chemical process can be expected to be very complicated, the USER2 model is more apt for the feasibility and operability analysis.

3. The process flow diagram is modified to accommodate the USER model. All the streams from which information is required to perform feasibility and operability calculations are duplicated by passing them through duplicator blocks. The original stream is allowed to continue along the flow in the flowsheet and the duplicate is sent to the User block. For example Figure A.1 shows the modified flowsheet of the hot and cold water system (See Chapter 5) to accommodate the USER block.
4. Since, ASPEN PLUS™ does not have the facility to set up control loops, manipulator blocks are used to manipulate the values of those streams which are a part of the control strategies (See Figure A.1). The manipulator blocks are assigned the desired multiplication factor with which the values of the stream (which are passing through the blocks) are multiplied and changed.
5. Either standard codes or user written codes to analyze each of the criteria are acquired and inserted into the USER model.
6. An input file is created by exporting the backup file. It is the input file where all changes are made for running alternate designs. The input data required to perform the calculations in the USER file is added to the input file.
7. The files given in Appendices C and D have the input and user files for the hot and cold water mixing system and the methyl chloride process respectively.

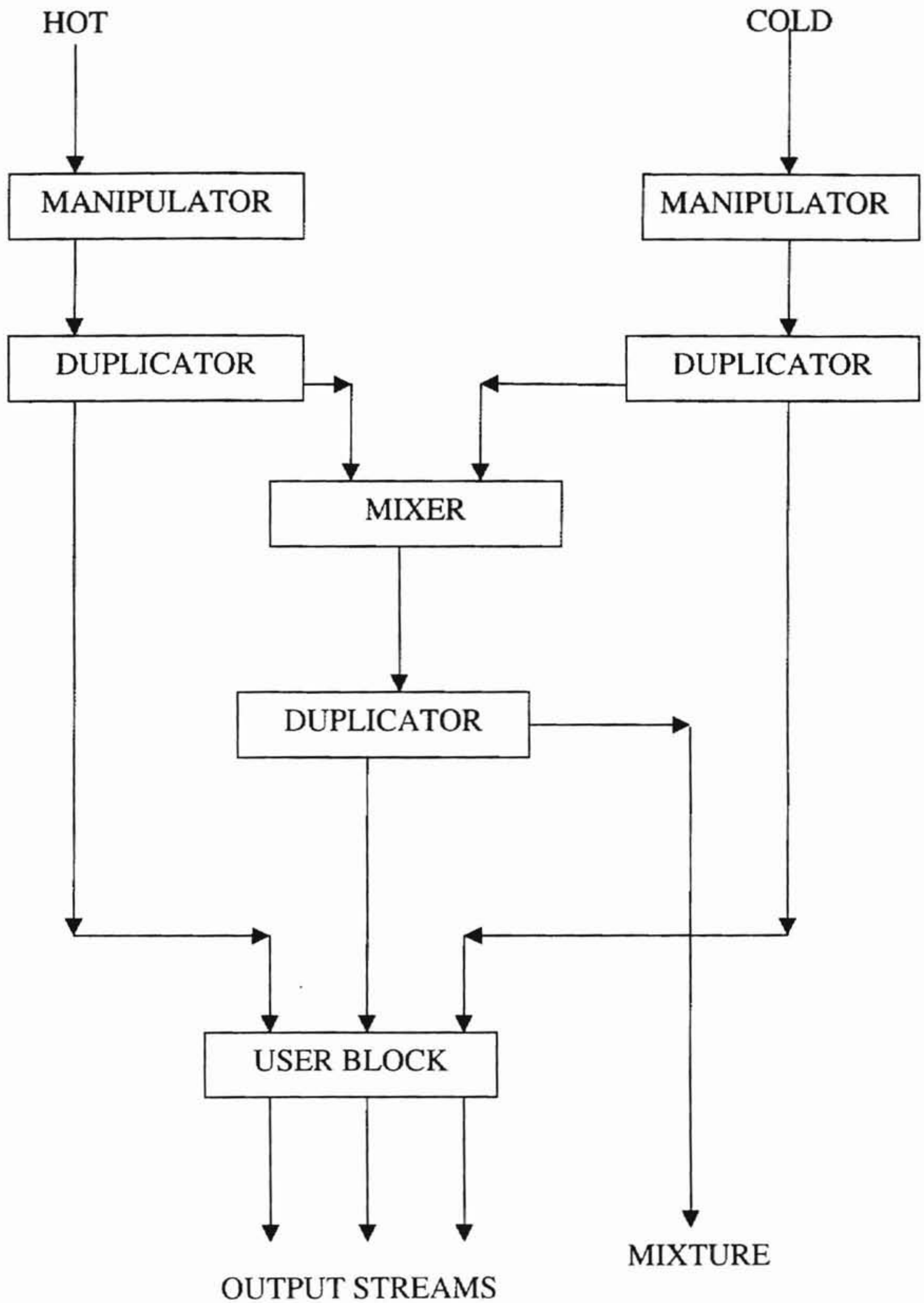


Figure A. 1 Hot and Cold Water System for Controllability Analysis

A.1.1 Controllability Analysis Specific to the Current Research Work

8. This section presents the steps followed to perform controllability analysis on the Methyl Chloride process.

   a) The controlled variables were the product flow rate, *PROD* and product purity, *XPRD*. The manipulated variables chosen were the feed flow rate, *FEED* and heat supply to the feed preheater, *HEATH*.

   b) The flow sheet is modified by sending the duplicates of the product, feed and heat streams to the USER block (See Figure A.2). The heat streams (*HEATH* and *HEATC*) are just indicators of carriers of the corresponding amount of heat as far as the design of the process is concerned. So, the information of the heat streams is sent to the USER block by using an information stream.

   c) To perform the singular value analysis, the gain matrix needs to be developed (See Chapter 3) for which the first step is to change the value of each manipulated variable (MV) at a time. This changes the values of the controlled variables (CV). The values of the elements of the gain matrix, K_{ij}, are calculated and stored in the corresponding data file. Now, for generating the gain matrix, first the multiplication factor, MVM1 (*MV = FEED*) is changed by the desired percentage. This changes the flowrate of the feed stream, *FEED*, to how much ever is desired.

   d) The "WRITE" statement to the data file for MV2 is commented in the user file (to avoid overwriting the K_{ij} values corresponding to a change in MVM2

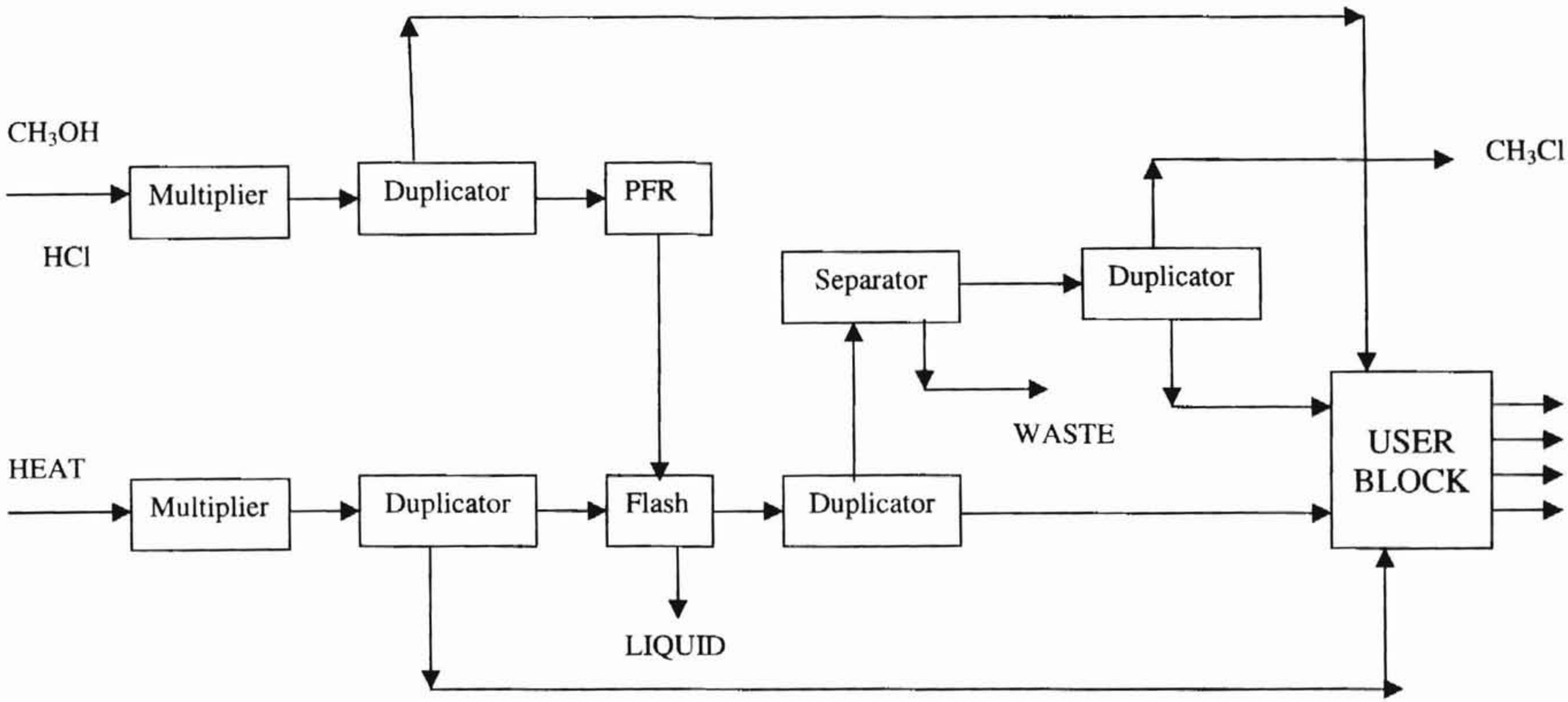


Figure A. 2 Methyl Chloride Process for Controllability Analysis

($MV=HEATH$)) and the simulation is run now (See Appendix D, Section D.2). The values of the first column of the matrix are calculated by Equation 3.4,

$$K_{ij} = \frac{(CV_i - CV_{iO})/CV_D}{(MV_1 - MV_{1O})/MV_{1D}} \qquad 3.4$$

and, get recorded in MV1.dat.

e) Next, MVM1 is changed back to 1.0 and MVM2 is now changed by the desired percentage in the input file. The "WRITE" statement to MV1.dat is commented in the user file (to avoid overwriting the K_{ij} values corresponding to a change in MVM1 ($MV=FEED$)) and the WRITE to MV2 .dat is uncommented out. K_{ij} values calculated by Equation 3.4 are now recorded in MV2.dat. These K_{ij} values correspond to the second column of the gain matrix.

f) The user file has statements to read the values of K_{ij} into the gain matrix, GKM from MV1.dat and MV2.dat. The program does that and the gain matrix is now ready to be subjected to singular value analysis, which is what follows in the user file. Thus, after step (e), the results would give the value of the condition number for that particular strategy.

g) The control strategy can be changed by assigning a different variable to MV_n or CV_n or both in the user file. For example, in the alternate strategy demonstrated in this work, MV2 was changed to heat supply to condenser, HEATC. The simulation is run again following steps (b) to (f) and the value of CN for the alternate strategy is obtained.

h) Alternate control strategies are then compared with the condition number. The strategy having the lower condition number gives better controllability to the process.

A.1.2 Environmental Impact Analysis Specific to this Work

9. This section gives the steps followed to perform environmental impact analysis on methyl chloride process.
    a) The calculation of environmental impact is quite straight forward. The values of the environmental impact index (See Table 6.4) are included in the input file in the Real Value list of the User block (See Section D.1).
    b) Environmental impact analysis calculates the impact of all chemicals in each stream in the process design. Duplicate blocks for the feed, vapor from flash chamber and product streams have already been created for controllability analysis (See Figure A.2). So, duplicate blocks are now installed for the remaining three streams. The duplicates of these streams are also sent to the USER block (See Figure A.3).
    c) The equation 3.6 is coded in the User file (See Section D.2).
    d) The simulation is run and the environmental impact value is generated.

A.1.3 Profitability Analysis Specific to this Work

10. This section deals with the steps followed to perform profitability analysis on the methyl chloride process.
    a) The calculation of Annual Equivalent Profit (AEP) also does not require any changes by the user during simulation. The values of the costs of the reactants and products are included in the Real Value list of the input file (See Section D.1).

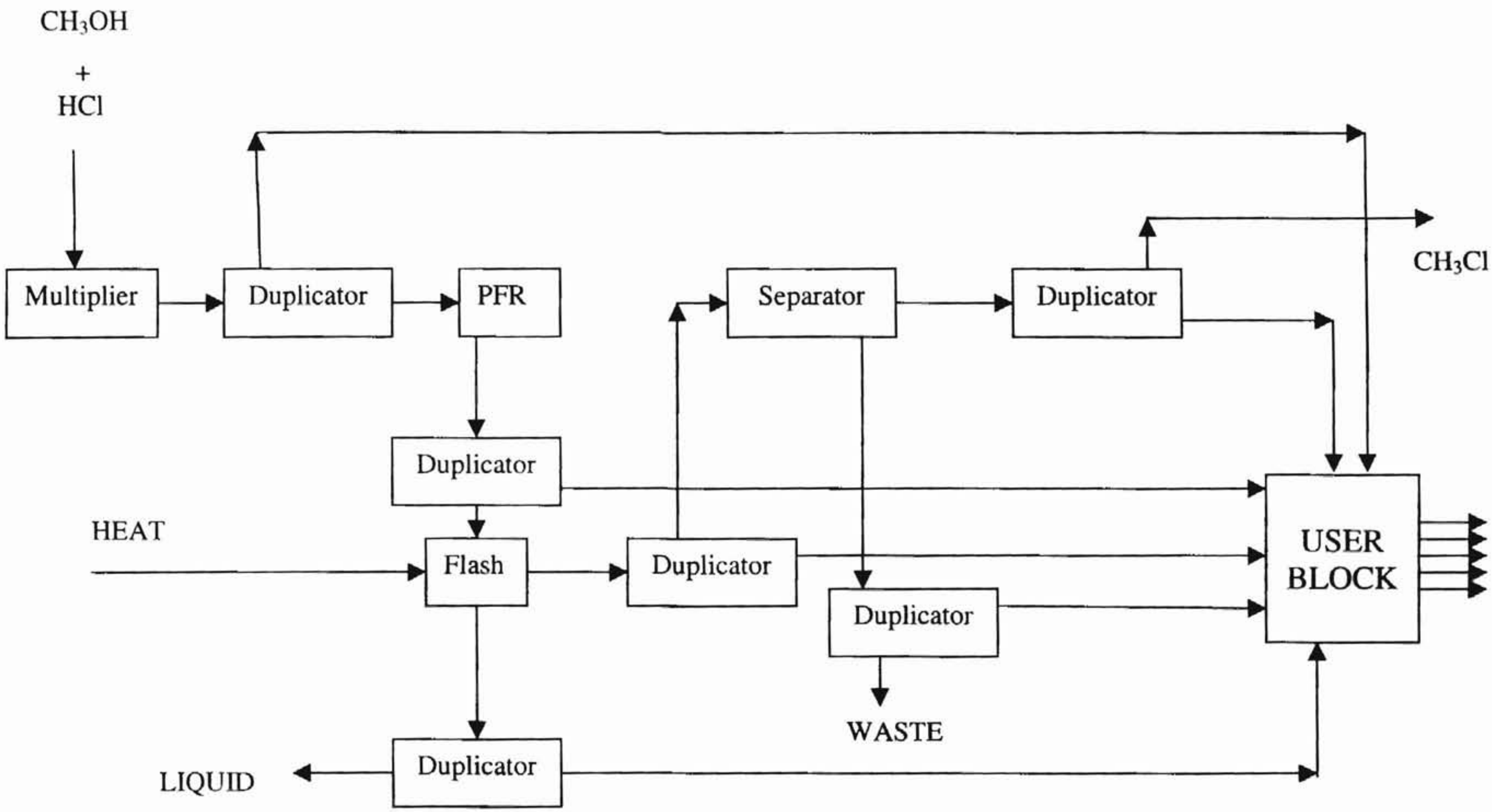


Figure A. 3 Methyl Chloride Process for Environmental Impact Analysis

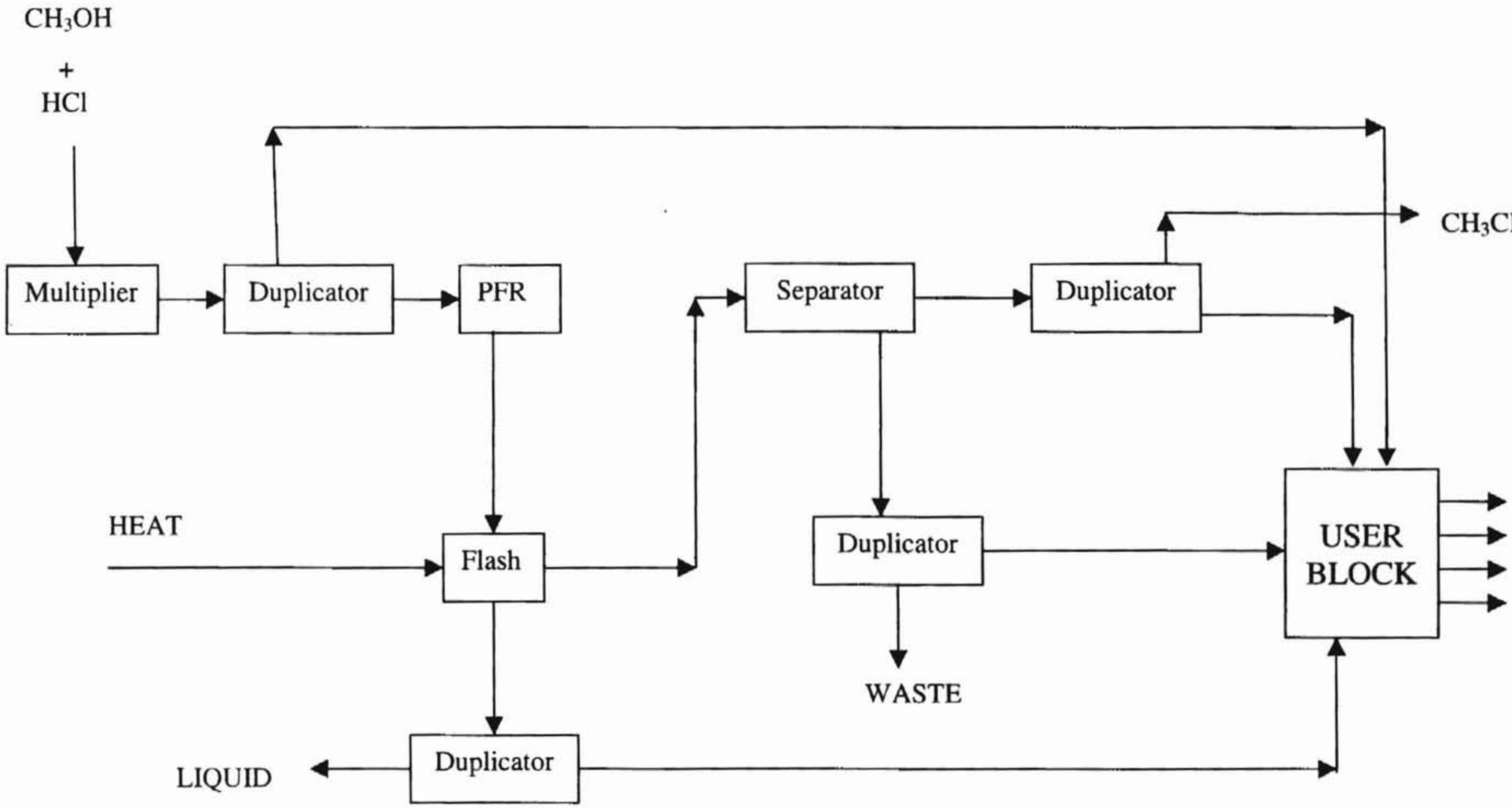


Figure A. 4 Methyl Chloride Process for Profitability Analysis

b) Profitability analysis requires information from the feed stream and the product and waste streams alone. Duplicates for these have already been prepared in the previous analyses. So, the flowsheet appears as shown in Figure A.4.

c) Equations 3.11 to 3.17 are coded in the USER file.

The simulation is run and the value of AEP is obtained for that design.

11. Individual analysis of controllability, environmental impact or profitability: If either of the three indices needs to be calculated for any design, say controllability, then the sections titled, environmental impact and profitability can be deleted and controllability run alone following step 7 to get the condition number and the same applies for environmental impact and profitability too (See Figures A.6, A.7 and A.8).

12. Combined analysis of controllability, environmental impact or profitability (See Figure A.4): If all three are to be calculated together for any design, then the user file given in Section D.2 can be used as such and run following steps 7 to 9 to give the values of all three indices.

13. Steps 1 to 11 are repeated for each alternate design.

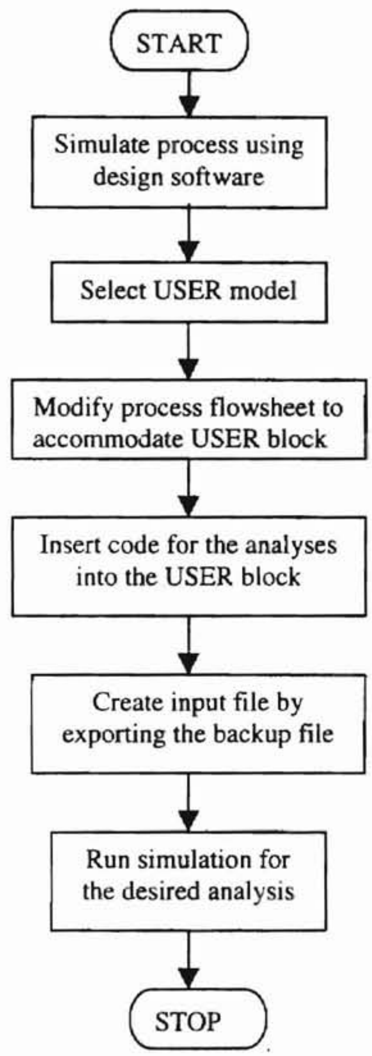


Figure A. 5 Flowsheet for Overall Operability Analysis

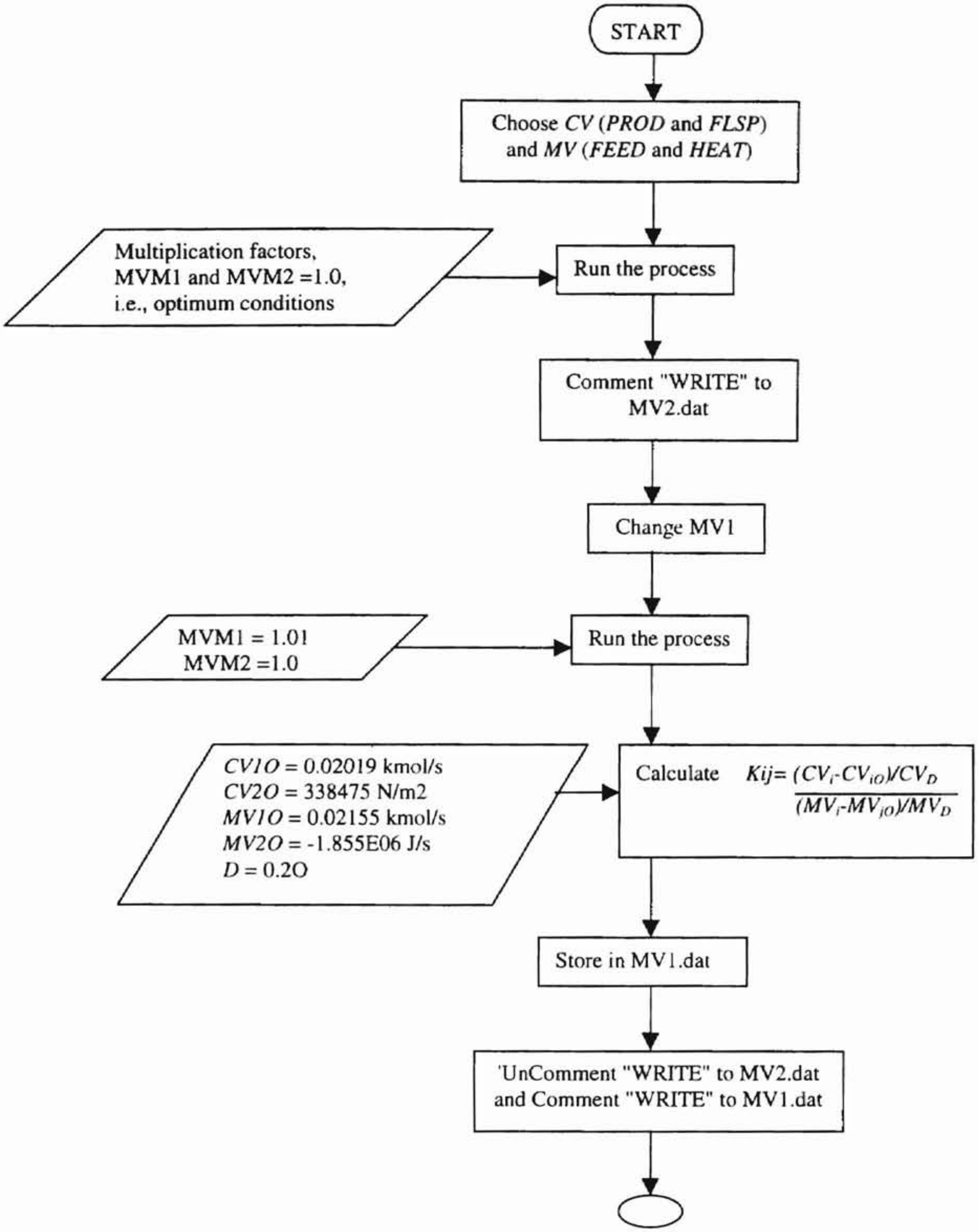


Figure A. 6 Flowsheet for Controllability Analysis

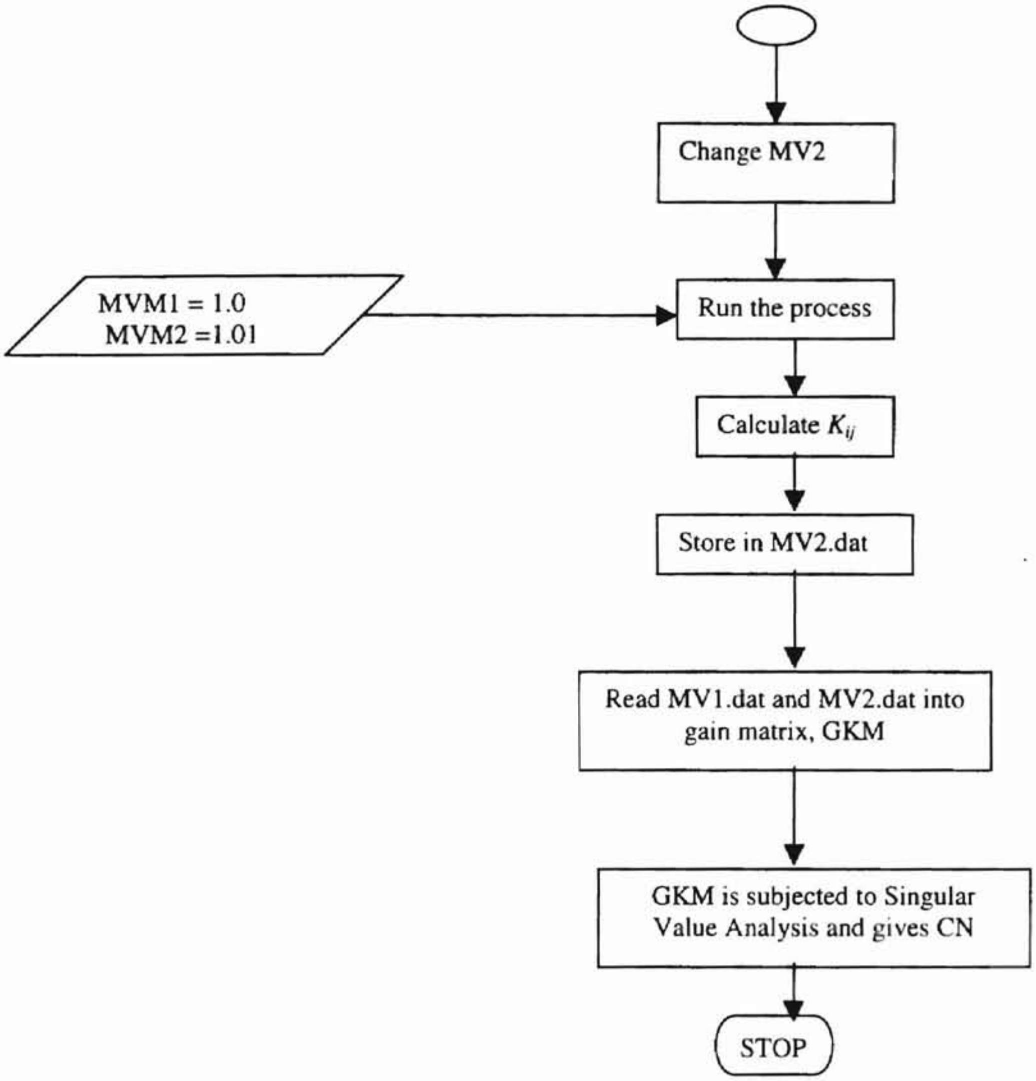


Figure A. 6 Flowsheet for Controllability Analysis, contd.

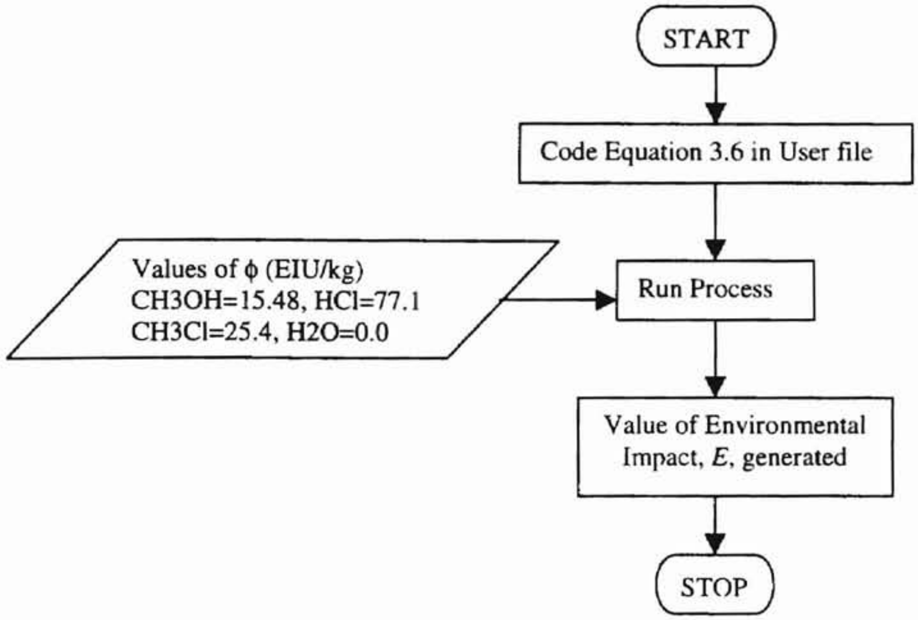


Figure A. 7 Flowsheet for Environmental Impact Analysis

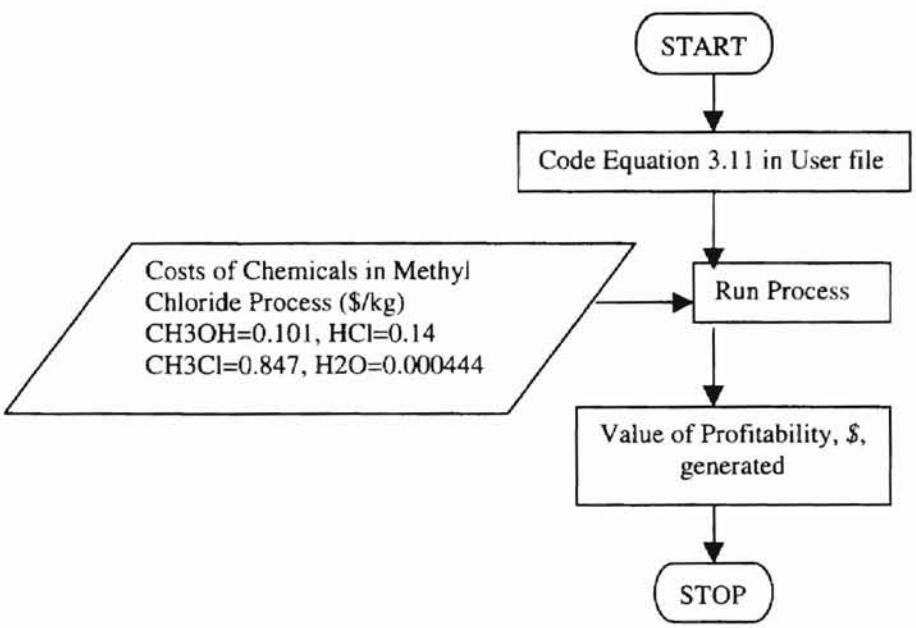


Figure A. 8 Flowsheet for Profitability Analysis

APPENDIX B

Calculations of Environmental Impact and Profitability for the Methyl Chloride Process

This Chapter describes the calculations and results obtained for the environmental impact and profitability of the methyl chloride process, which were discussed in Chapter 6. This Chapter is intended to supply the details required to make similar calculations for any alternate designed. For demonstration purposes, calculations for Alternate 1, which uses an adiabatic PFR are discussed.

B.1 Environmental Impact Calculations

Environmental impact is calculated by Equation 3.6:

$$E = \frac{\sum_{i=1}^{n}\sum_{j=1}^{m} r_i w_i m_{j,i} \phi_j}{P} \qquad 3.6$$

where, r_i (release factor of stream i) is assumed to be equal to 1.0 for all streams,

w_i (total mass flowrate of stream i) is obtained from ASPEN simulations,

$m_{j,i}$ (mass fraction of each component j in stream i), also obtained from ASPEN simulations,

ϕ_j (environmental impact index of the chemical j), obtained from standard data

and, P (product flow rate), obtained from ASPEN simulations.

Table 6.5 shows the results obtained for the environmental impact of the methyl chloride process for the three designs. From Table 6.5, the environmental impact of Alternate 1 (which uses an adiabatic PFR) is 362.0 EIU/kg. The following section demonstrates how this result has been achieved.

The streams involved in these calculations are: 1) Feed to adiabatic PFR. 2) Adiabatic PFR to Condenser. 3) Condenser to flash. 4) Vapor stream from flash. 5) Liquid waste from flash. 6) Product from separator. 7) Waste from separator. The environmental impact indices in EIU/kg from Table 6.4 are: $\phi_{CH3OH} = 15.48$, $\phi_{CH3Cl} =$

77.1, $\phi_{HCl} = 25.4$. From the process flow diagram in Figure 6.3, the flowrates of streams and mass fractions of components in the streams are as given in Table B.1.

Table B.1 Mass Flowrate (w_i) of Stream i and Mass Fraction ($m_{j,i}$) of Component j in Stream i

Stream (i)	Feed	PFR Product	Condenser to Flash	Flash Vapor	Flash Liquid	Product	Separator Waste
Mass flow rate (wi, kg/s)	1.37	1.37	1.37	1.32	0.047	0.63	0.69
m_{CH3OH}	0.47	0.173	0.173	0.171	0.225	0.0	7.07E-3
m_{HCl}	0.53	0.197	0.197	0.203	0.015	0.0	7.38E-3
m_{CH3Cl}	0.0	0.464	0.464	0.478	0.094	1.0	1.25E-5
m_{H2O}	0.0	0.166	0.166	0.148	0.666	0.0	0.011

In Equation 3.6, P = 0.63kg/s (product flowrate obtained). For each stream, the quantity $\sum_{j=1}^{4} (r_i w_j m_{j,i} \phi_j)$ needs to be calculated. Taking product stream from PFR as example:

$$\sum_{j=1}^{4} (r_i w_j m_{j,i} \phi_j) = 1.0 \times 1.37 \times (0.173 \times 15.48 + 0.197 \times 77.1 + 0.464 \times 25.4 + 0.166 \times 0.0) = 40.62$$

Similar calculations are performed for other streams and the results are given in Table B.2.

Table B. 2 Environmental Impact of Streams in Methyl Chloride Process

Stream (i)	$\sum_{j=1}^{4} (r_i w_j m_{j,i} \phi_j)$ (EIU)
Feed	66.12
PFR product	40.62
Condenser to Flash	40.62
Flash Vapor	40.24
Flash Liquid	0.33
Product	16.03
Separator Waste	24.29
$\sum_{i=1}^{7} \sum_{j=1}^{4} (r_i w_j m_{j,i} \phi_j)$	228.25

The value in the last row is the sum of the environmental impact values of all streams.

The product flow rate from the product stream (P) = 0.63kg/s

Therefore, E = 228.25/0.63 = 362.0 EIU/kg. Thus, the environmental impact of alternate 1 is 362.0 EIU/kg.

B.2 Profitability Calculations

Profitability of the process is calculated by Equations 3.11 to 3.17. The calculation of cash flow of the process requires the evaluation of cash inflow and cash outflow.

CF_i = Cash Inflow or, the revenue obtained from the products generated as a result of the process.

CF_o = Cash Outflow, or all the costs involved in the process

The results for profitability analysis of the methyl chloride process are given in Table 6.8. From that, the AEP of alternate 1 is 2.48M$/yr. The following sections demonstrate the calculations involved to obtain this result.

From Table 6.7 (costs of the products (CH_3Cl and H_2O) are: 0.847 and 0.00044 $/kg) and Table B.1 (flowrates and compositions of streams):

CF_i = 0.63 x 1.0 x 0.847 + 0.63 x 0.0 x 0.00044 = 0.534$/s = 16.9M$/yr

Following section describes the costs that contribute to cash outflow.

B.2.1 Costs included in cash out flow

The costs included in CF_o are given below:

Raw material costs

From Table 6.7, costs of the raw materials are:

CH_3OH = 0.101$/kg and HCl = 0.14$/kg.

From Table B.1, the flowrates of the raw materials are:

$CH_3OH = w_{feed} \times m_{CH3OH}$ = 1.37 x 0.47 = 0.644kg/s

HCl $= w_{feed} \times m_{HCl}$ = 1.37 x 0.53 = 0.726kg/s

Raw material cost = 0.644 x 0.101 + 0.726 x 0.14 = 0.167$/s = 5.26M$/yr

Utilities Costs

Preheating duty (from ASPEN runs) = 1.195E6 J/s

Cooling water flow rate (from ASPEN runs) = 0.9975kg/s

From Table 6.7 utilities costs are: Preheating cost = 3.03E-9$/J

Cooling water cost = 7.3E-5 $/kg

Hence, Utilities costs = 1.195E6 x 3.03E-9 + 0.9975 x 7.3E-5 = 3.693E-3 \$/s = 0.117M\$/yr

Waste treatment costs

This is the cost involved in the treatment of waste streams, liquid flash and separator waste. From Table 6.7, treatment cost = 0.50/kg organic mass.

Organic mass = Mass of CH_3OH and CH_3Cl present in the waste streams (from Table B.1): 0.047x(0.225+0.094) + 0.69 x (7.07E-3 + 1.25E-5) = 0.242kg/s

Treatment costs = 0.242x0.50 = 0.121 \$/s =3.82M\$/yr

Waste disposal costs

Waste disposal costs are calculated by \$/kg waste. From Table 6.7, the disposal costs = 0.165 \$/kg waste.

Thus, waste disposal costs = (0.047 + 0.69) x 0.165 = 0.122 \$/s = 3.85M\$/yr

Cash Outflow

Cash outflow, as mentioned earlier is a sum of all the costs involved. Therefore,

CF_o = 0.41 \$/s = 13.04M\$/yr

Depreciation (Equation 3.13)

Depreciation is calculated by the straight line depreciation method. Thus,

$F_d = F_c/N_y$ = 19500/5 = \$3900 = 3.9E-3 M\$/yr

Taxable Income (Equation 3.14)

$$TI = CF_i - CF_o - F_d \quad (3.14)$$

$$= 16.9 - 13.04 - 3.9E\text{-}3$$

$$= 3.86M$$

Net Income (Equation 3.15)

Cash Flow (Equation 3.1

Finally, cash flow is the

For n = 0, cash flow is co

$CF_0 = F_c + W_c = \$19500$

NPV is calculated using I

Annual worth factor is cal

Now, AEP is calculated by

Thus, the annual equivalen

APPENDIX C

INPUT AND USER FILES FOR HOT AND COLD WATER SYSTEM

C.1 Input File for the Hot and Cold Water Mixing System

```
TITLE 'CONTINUOUS MIXING SYSTEM OF HOT AND COLD WATER'

; Input file for the design of the hot and cold water mixing system and the development
; of singular value analysis.

IN-UNITS ENG

OUT-UNITS SI

DEF-STREAMS CONVEN ALL

DATABANKS PURECOMP / AQUEOUS / SOLIDS / INORGANIC / &
    NOASPENPCD

PROP-SOURCES PURECOMP / AQUEOUS / SOLIDS / INORGANIC

COMPONENTS
  H2O H2O H2O

FLOWSHEET
  BLOCK MIXER IN=SHO SCO OUT=MIXTURE
  BLOCK USER IN=SHD SCD SMD OUT=10 14 15
  BLOCK HD IN=12 OUT=SHD SHO
  BLOCK CD IN=13 OUT=SCO SCD
  BLOCK MD IN=MIXTURE OUT=8 SMD
  BLOCK HM IN=HOT OUT=12
  BLOCK CM IN=COLD OUT=13

PROPERTIES RK-SOAVE

STREAM COLD
  SUBSTREAM MIXED TEMP=65.0 PRES=14.6959488
  MOLE-FLOW H2O 555.564903

STREAM HOT
  SUBSTREAM MIXED TEMP=100.0 PRES=14.6959488
  MOLE-FLOW H2O 277.782452

BLOCK MIXER MIXER

; Following are the Multiplier blocks used to manipulate the flowrates of the hot and
; cold water streams. The multiplying factor can be changed by the desired amount.
```

```
; Manipulator for the cold water stream
BLOCK CM MULT
  PARAM FACTOR=1.0

; Manipulator for the hot water stream
BLOCK HM MULT
  PARAM FACTOR=1.01

; DUPL blocks are used to duplicate the stream and send to the USER block where SVA
; is performed.

; Duplicator for cold water stream
BLOCK CD DUPL

; Duplicator for hot water stream
BLOCK HD DUPL

; Duplicator for mixture stream
BLOCK MD DUPL

BLOCK USER USER2
  IN-UNITS SI
  SUBROUTINE USRHCS
  PARAM NINT=2 NREAL=9
  INT VALUE-LIST=2

; List of initial steady state optimum values and maximum acceptable deviations of
; controlled and manipulated variables from initial values

  REAL VALUE-LIST=.0350 .070 .1050 297.95880 .0070 .0140 &
    .0210 59.5920

CONV-OPTIONS
  PARAM CHECKSEQ=NO
```

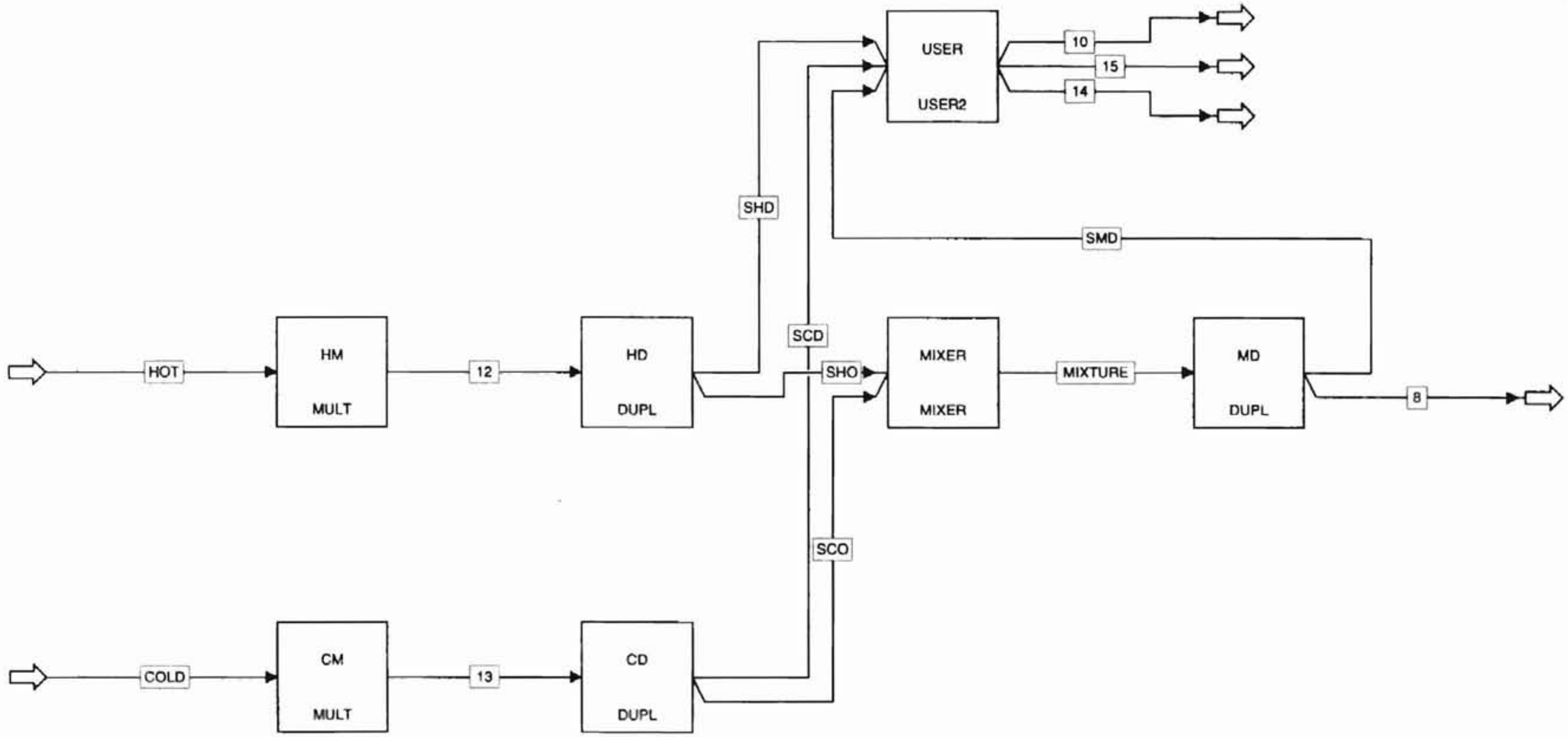


Figure C. 1 Aspen Flow Diagram for the Hot and Cold Water Mixing System

C.2 User file for the Hot and Cold Water Mixing System

```
C    User Unit Operation Model (or Report) Subroutine for USER2
C    User routine to perform Singular Value Decomposition to find the singular
C    values and hence, the Condition Number of the hot and cold water mixing
C    system.

      SUBROUTINE USRHCS (NMATI, SIN,   NINFI,  SINFI, NMATO,
     2             SOUT,  NINFO, SINFO,  IDSMI, IDSII,
     3             IDSMO, IDSIO, NTOT.   NSUBS, IDXSUB,
     4             ITYPE, NINT,  INT,    NREAL, REAL,
     5             IDS,   NPO,   NBOPST, NIWORK, IWORK,
     6             NWORK, WORK,  NSIZE,  SIZE,  INTSIZ,
     7             LD)
C
      IMPLICIT REAL*8 (A-H, O-Z)
C
      COMMON /USER/ RMISS,  IMISS,  NGBAL, IPASS, IRESTR,
     2           ICONVG, LMSG,   LPMSG, KFLAG, NHSTRY,
     3           NRPT,   NTRMNL, ISIZE

C
      DIMENSION SIN(NTOT,NMATI), SINFI(NINFI), SOUT(NTOT,NMATO),
     2       SINFO(NINFO), IDSMI(2,NMATI), IDSII(2,NINFI),
     3       IDSMO(2,NMATO), IDSIO(2,NINFO), IDXSUB(NSUBS),
     4       ITYPE(NSUBS), INT(NINT), REAL(NREAL), IDS(2,3),
     5       NBOPST(6,NPO), IWORK(NIWORK), WORK(NWORK),
     6       SIZE(NSIZE), INTSIZ(NSIZE)

C
      COMMON /NCOMP/ NCC

      DIMENSION CMV(20), CV(20), aMV(20), v(20,20), w(20), rv1(20)
      DIMENSION GKM(20,20)

C   Opening the files in which the values of the elements of the gain matrix are
C   temporarily stored, between the manipulations of the manipulated variables.

C   SIMC.DAT is for storing elements of the gain matrix when the cold water flow rate
C   is manipulated.

      OPEN (UNIT=1, FILE="SIMC.DAT", STATUS="OLD")

C   SIMH.DAT is for storing elements of the gain matrix when the hot water flow rate is
C   manipulated.
```

```
      OPEN (UNIT=2, FILE="SIMH.DAT", STATUS="OLD")

C     Storing values of inlet material strams to outlet material streams

      DO 100 I = 1, NTOT
        DO 50 J=1,NTOT
          SOUT(I,J) = SIN(I,J)
 50     CONTINUE
100   CONTINUE

C     Number of controlled (manipulated) variables or dimensions of the Gain matrix.
C     Here, NV = 2.  Value of INT(1) mentioned in the input file.

      NV = INT(1)

C     Optimum values of MV and CV
      FHO = REAL(1)
      FCO = REAL(2)
      FMO = REAL(3)
      TMO = REAL(4)

C     Ranges of CV and MV
      FHR = REAL(5)
      FCR  = REAL(6)
      FMR = REAL(7)
      TMR = REAL(8)

C     Following are the expressions to calculate the physically scaled values of each
C     manipulated and controlled variable.
C     The expressions are obtained from Equation 3.4.

      CV(1)=(SOUT(3,3)-TMO)/TMR
      CV(2)=(SOUT(1,3)-FMO)/FMR
      aMV(1)=(SOUT(1,2)-FCO)/FCR
      aMV(2)=(SOUT(1,1)-FHO)/FHR

C     Calculation of the elements of the gain matrix (GKM()).  Each element is defined as
C     the ratio of the physically scaled value of the controlled variable to that of the
C     manipulated variable.  These values are obtained by alternately commenting out the
C     WRITE statements to file 1 and 2.  When WRITE to file2 is commented (as shown
C     below), then  cold water flowrate is manipulated and the corresponding elements of
C     the gain matrix are recorded in File 1 SIMC.DAT).  Then WRITE to file 1 is
C     commented, hot water flowrate is manipulated and the corresponding elements of the
C     gain matrix are recorded in File 2 (SIMH.DAT).

      DO 10 I=1,NV
```

```
      DO 5 J=1,NV
C   Elements of the first row of the gain matrix (Equation 3.4).
      CMV(1)= CV(J)/aMV(1)
      WRITE(1, *) CMV(1)
C   Elements of the second row of the gain matrix (Equation 3.4).
      CMV(2)= CV(J)/aMV(2)
C       WRITE(2, *) CMV(2)
  5    CONTINUE
      CLOSE(1)
      CLOSE(2)
 10  CONTINUE

C   Gain matrix values are read back into the gain matrix, GKM(), from the files 1 and 2.

     DO 102 I=1,NV
      OPEN(UNIT=1, FILE="SIMC.DAT",STATUS="OLD")
      READ(1,*,END=777)GKM(I,1)
102   CONTINUE

777   DO 103 I=1,NV
      OPEN(UNIT=2, FILE="SIMH.DAT",STATUS="OLD")
      READ(2,*,END=888)GKM(I,2)
103   CONTINUE

 30  FORMAT(5X, F16.8)

    WRITE(NRPT,*)"Elements of the gain matrix"
    DO 105 I=1,NV
      DO 104 J=1,NV
      WRITE(NRPT,55)GKM(I,J)
104 CONTINUE
105 CONTINUE

C  Singular Value Analysis to find best control strategy
C  Source:  Numerical Recipes in Fortran, 2nd Ed.
C  Control strategy being tested: Fc - Tm; Fh - Fm
C  This routine computes the singular value decomposition of the gain matrix as
C  GKM = U. W. V^T.

888 n=NV
    m=NV

C  House holder reduction to bidiagonal form.
    g=0.0
    scale=0.0
    anorm=0.0
```

```
      do 25 i=1,n
        l=i+1
        rv1(i)=scale*g
        g=0.0
        s=0.0
        scale=0.0
        if(i.le.m)then
          do 11 k=i,m
            scale=scale+abs(GKM(k,i))
11        continue
          if(scale.ne.0.0)then
            do 12 k=i,m
              GKM(k,i)=GKM(k,i)/scale
              s=s+GKM(k,i)*GKM(k,i)
12          continue
            f=GKM(i,i)
            g=-sign(sqrt(s),f)
            h=f*g-s
            GKM(i,i)=f-g
            do 15 j=l,n
              s=0.0
              do 13 k=i,m
                s=s+GKM(k,i)*GKM(k,j)
13            continue
              f=s/h
              do 14 k=i,m
                GKM(k,j)=GKM(k,j)+f*GKM(k,i)
14            continue
15          continue
            do 16 k=i,m
              GKM(k,i)=scale*GKM(k,i)
16          continue
          endif
        endif
        w(i)=scale *g
        g=0.0
        s=0.0
        scale=0.0
        if((i.le.m).and.(i.ne.n))then
          do 17 k=l,n
            scale=scale+abs(GKM(i,k))
17        continue
          if(scale.ne.0.0)then
            do 18 k=l,n
              GKM(i,k)=GKM(i,k)/scale
```

```
          s=s+GKM(i,k)*GKM(i,k)
 18       continue
        f=GKM(i,l)
        g=-sign(sqrt(s),f)
        h=f*g-s
        GKM(i,l)=f-g
        do 19 k=l,n
          rv1(k)=GKM(i,k)/h
 19       continue
        do 23 j=l,m
          s=0.0
          do 21 k=l,n
            s=s+GKM(j,k)*GKM(i,k)
 21         continue
          do 22 k=l,n
            GKM(j,k)=GKM(j,k)+s*rv1(k)
 22         continue
 23       continue
        do 24 k=l,n
          GKM(i,k)=scale*GKM(i,k)
 24       continue
       endif
      endif
      anorm=max(anorm,(abs(w(i))+abs(rv1(i))))
 25  continue

 C  Accumulation of right hand transformations

    do 32 i=n,1,-1
      if(i.lt.n)then
       if(g.ne.0.0)then

C  Double division to avoid possible underflow
         do 26 j=l,n
          v(j,i)=(GKM(i,j)/GKM(i,l))/g
 26       continue
        do 29 j=l,n
          s=0.0
          do 27 k=l,n
            s=s+GKM(i,k)*v(k,j)
 27         continue
          do 28 k=l,n
            v(k,j)=v(k,j)+s*v(k,i)
 28         continue
 29       continue
       endif
```

```
        do 31 j=l,n
          v(i,j)=0.0
          v(j,i)=0.0
 31     continue
      endif
      v(i,i)=1.0
      g=rv1(i)
      l=i
 32 continue

C Accumulation of left hand transformations
    do 39 i=min(m,n),1,-1
      l=i+1
      g=w(i)
      do 33 j=l,n
        GKM(i,j)=0.0
 33   continue
      if(g.ne.0.0)then
        g=1.0/g
        do 36 j=l,n
          s=0.0
          do 34 k=l,m
            s=s+GKM(k,i)*GKM(k,j)
 34       continue
          f=(s/GKM(i,i))*g
          do 35 k=i,m
            GKM(k,j)=GKM(k,j)+f*GKM(k,i)
 35       continue
 36     continue
        do 37 j=i,m
          GKM(j,i)=GKM(j,i)*g
 37     continue
      else
        do 38 j= i,m
          GKM(j,i)=0.0
 38     continue
      endif
      GKM(i,i)=GKM(i,i)+1.0
 39 continue


C Diagonalization of the bidiagonal form:  Loop over singular values, and over allowed
C iterations.
    do 49 k=n,1,-1
      do 48 its=1,30
```

```
C  Test for splitting
        do 41 l=k,1,-1
          nm=l-1
          if((abs(rv1(l))+a
          if((abs(w(nm))+
 40  continue

C  Cancellation of rv1(l),
 1        c=0.0
        s=1.0
        do 43 i=l,k
          f=s*rv1(i)
          rv1(i)=c*rv1(i)
          if((abs(f)+anorm
            g=w(i)
c           h=pythag(f,g)
            h=DSQRT(DA
            w(i)=h
            h=1.0/h
            c= (g*h)
            s=-(f*h)
            do 42 j=1,m
              y=GKM(j,nm
              z=GKM(j,i)
              GKM(j,nm)=(
              GKM(j,i)=-(y
 42           continue
 43       continue
 2        z=w(k)

C  convergence
        if(l.eq.k)then

C  Singular value is made 
          if(z.lt.0.0)then
            w(k)=-z
            do 44 j=1,n
              v(j,k)=-v(j,k)
 44           continue
          endif
          goto 3
        endif
        WRITE(10,*)"its="
        WRITE(10,*)its
        if(its.eq.30) pause 'r
```

```
C  Shift from bottom 2-by-2 minor.
         x=w(l)
         nm=k-1
         y=w(nm)
         g=rv1(nm)
         h=rv1(k)
         f=((y-z)*(y+z)+(g-h)*(g+h))/(2.0*h*y)
c        g=pythag(f,1.0)
         g=DSQRT(DABS(f**2)+1.0)
         WRITE(10,*)"g"
         WRITE(10,*)g
         f=((x-z)*(x+z)+h*((y/(f+sign(g,f)))-h))/x

C  Next QR transformation.
         c=1.0
         s=1.0
         do 47 j=l,nm
           i=j+1
           g=rv1(i)
           y=w(i)
           h=s*g
           g=c*g

C  Pythagoros function
           z=DSQRT(DABS(f**2)+DABS(h**2))
           rv1(j)=z
           c=f/z
           s=h/z
           f= (x*c)+(g*s)
           g=-(x*s)+(g*c)
           h=y*s
           y=y*c
           do 45 jj=1,n
             x=v(jj,j)
             z=v(jj,i)
             v(jj,j)= (x*c)+(z*s)
             v(jj,i)=-(x*s)+(z*c)
 45        continue
           z=DSQRT(DABS(f**2)+DABS(h**2))

C  Rotation can be arbitraryif z = 0.
           w(j)=z
           if(z.ne.0.0)then
             z=1.0/z
             c=f*z
```

```
        s=h*z
      endif
      f= (c*g)+(s*y)
      x=-(s*g)+(c*y)
      do 46 jj=1,m
        y=GKM(jj,j)
        z=GKM(jj,i)
        GKM(jj,j)= (y*c)+(z*s)
        GKM(jj,i)=-(y*s)+(z*c)
46      continue
47    continue
    rv1(l)=0.0
    rv1(k)=f
    w(k)=x
48  continue
 3  continue
49 continue
```

C Printing values of the U (Left Singular Vector) array.

```
   WRITE(NRPT,*)"Elements of U"
   do 56 i=1,m
     do 51 j=1,n
       WRITE(NRPT,60)GKM(i,j)
51   continue
56 continue
```

C Printing values of V (Right Singular Vector) array.

```
   WRITE(NRPT,*)"Elements of V"
   do 57 i=1,m
     do 53 j=1,n
       WRITE(NRPT,60)v(i,j)
53   continue
57 continue
```

C Printing singular values of the matrix

```
   WRITE(NRPT,*)"Singular Values of the Gain Matrix"
   do 52 i=1,n
     WRITE(NRPT,55)w(i)
     WRITE(10,55)w(i)
52 continue
```

C Sorting the array of singular values to arrange it in increasing order.

```
      do 503 j=2,n
        a=w(j)
        do 500 i=j-1,1,-1
          if(w(i).le.a)goto 502
          w(i+1)=w(i)
500       continue
        i=0
502       w(i+1)=a
503   continue

      WRITE(NRPT,*)"Sorted array of singular values"
      do 504 i=1,n
        WRITE(NRPT,55)w(i)
504   continue

C     Calculation of the condition number.  It is the ratio of the max (singular value) to the
C     min (singular value) (Equation 3.5).

      CN=w(N)/w(1)
      WRITE(NRPT,*)"CN="
      WRITE(NRPT,55)CN

 55   FORMAT(F8.4)
 60   FORMAT(F10.6)

999   RETURN
      END
```

APPENDIX D

INPUT AND USER FILES FOR METHYL CHLORIDE PROCESS

D.1 Input File for the Methyl Chloride Process

```
TITLE 'METHYL CHLORIDE PRODUCTION'

; This is a simplified version of the methyl chloride process. SVA for controllability
; analysis, and environmental impact analysis are done.
; Used information streams to send information (heat duty) of the heat stream to the user
;  block.

TITLE 'METHYL CHLORIDE PRODUCTION'

IN-UNITS ENG

OUT-UNITS SI

DEF-STREAMS CONVEN ALL

SIM-OPTIONS FLASH-MAXIT=50 FLASH-TOL=.0010

RUN-CONTROL MAX-TIME=15000.0 MAX-ERRORS=1000000 &
    MAX-FORT-ERR=100000

DESCRIPTION "THIS RUN INCLUDES THE SUPERSTRUCTURE WITH ALL
POSSIBLE
    ALTERNATIVES "

DATABANKS AQUEOUS  / ASPENPCD  / PURECOMP  / SOLIDS  / &
    INORGANIC

PROP-SOURCES AQUEOUS  / ASPENPCD  / PURECOMP  / SOLIDS  / &
    INORGANIC

COMPONENTS
  H2O H2O H2O /
  HCL HCL HCL /
  CH3CL CH3CL CH3CL /
  CH3OH CH4O CH3OH

COMP-GROUP G2 SUBSTREAM=MIXED COMPS=HCL CH3CL

COMP-GROUP G3 SUBSTREAM=MIXED COMPS=HCL CH3CL CH3OH H2O

FLOWSHEET
  BLOCK PFR IN=HTR-PFR OUT=PFRPROD
  BLOCK FLASH IN=CND-FLS1 OUT=VAPFL LIQFL
  BLOCK B29 IN=VAPFL-D1 OUT=PRODT W5
```

```
  BLOCK B3 IN=HCL-OHD2 PRODT-D2 VAPFL-D2 PFRPROD2 LIQFL-D2 &
    W5-D2 CND-FLS2 QH-HTR-2 QC-CND-2 OUT=23 25 26 27 28 &
    29 39 37 38
  BLOCK MVM1 IN=HCL-OH OUT=1
  BLOCK DUPL1 IN=1 OUT=HCL-OHD2 33
  BLOCK DUPL2 IN=PRODT OUT=PRODT-D1 PRODT-D2
  BLOCK MVM2 IN=QH OUT=QH-HTR
  BLOCK DUPL3 IN=VAPFL OUT=VAPFL-D1 VAPFL-D2
  BLOCK DUPL4 IN=QH-HTR OUT=QH-HTR-2 QH-HTR-1
  BLOCK DUPL5 IN=PFRPROD OUT=PFRPROD2 30
  BLOCK DUPL6 IN=LIQFL OUT=LIQFL-D1 LIQFL-D2
  BLOCK DUPL7 IN=W5 OUT=W5-D1 W5-D2
  BLOCK B1 IN=30 QC-CND-1 OUT=CND-FLS
  BLOCK B2 IN=33 QH-HTR-1 OUT=HTR-PFR
  BLOCK B4 IN=QC OUT=QC-CND-2 QC-CND-1
  BLOCK B5 IN=CND-FLS OUT=CND-FLS1 CND-FLS2

PROPERTIES NRTL-RK

STREAM HCL-OH
  IN-UNITS SI
  SUBSTREAM MIXED TEMP=300.0 PRES=101325.0
  MOLE-FLOW HCL .020 / CH3OH .020

DEF-STREAMS HEAT 37

DEF-STREAMS HEAT 38

DEF-STREAMS HEAT QC

STREAM QC
  IN-UNITS SI
  INFO HEAT DUTY=-1.000E+06

DEF-STREAMS HEAT QC-CND-1

DEF-STREAMS HEAT QC-CND-2

DEF-STREAMS HEAT QH

STREAM QH
  IN-UNITS SI
  INFO HEAT DUTY=1195000.0

DEF-STREAMS HEAT QH-HTR
```

```
DEF-STREAMS HEAT QH-HTR-1

DEF-STREAMS HEAT QH-HTR-2

BLOCK B29 SEP
   FRAC STREAM=PRODT SUBSTREAM=MIXED COMPS=H2O HCL CH3CL  &
      CH3OH FRACS=0.0 0.0 .9990 0.0

BLOCK B1 HEATER
   PARAM PRES=0.0

BLOCK B2 HEATER
   PARAM PRES=0.0

BLOCK FLASH FLASH2
   PARAM TEMP=213.47140 DUTY=0.0

BLOCK PFR RPLUG
   PARAM TYPE=ADIABATIC LENGTH=2.0 DIAM=1.0
   REACTIONS RXN-IDS=RSCH-2

CBLOCK E-2 HEATX
   SIZING-DATA TIN-TUBE=1200 <K> TOUT-TUBE=600 <K>
   REFERENCE SHELL BLOCK=B2

CBLOCK E-4 HEATX
   SIZING-DATA TIN-TUBE=160 <K> TOUT-TUBE=430 <K>
   REFERENCE SHELL BLOCK=B1

CBLOCK E-1 H-VESSEL
   SIZING-DATA DIAM=1 TT-LENGTH=2
   REFERENCE BLOCK=PFR

CBLOCK E-3 V-VESSEL
   SIZING-DATA RETEN-TIME=3 <MIN>
   REFERENCE BLOCK=FLASH

; Following are the Multiplier blocks used to manipulate the manipulated
; variables.  The multiplying factor can be changed by the desired amount.

BLOCK MVM1 MULT
   PARAM FACTOR=1.0

BLOCK MVM2 MULT
   PARAM FACTOR=1.0
```

```
BLOCK B4 DUPL

BLOCK B5 DUPL

; DUPL blocks are used to duplicate the stream and send to the USER block where SVA
is
; performed.

BLOCK DUPL1 DUPL

BLOCK DUPL2 DUPL

BLOCK DUPL3 DUPL

BLOCK DUPL4 DUPL

BLOCK DUPL5 DUPL

BLOCK DUPL6 DUPL

BLOCK DUPL7 DUPL

BLOCK B3 USER2
   IN-UNITS SI
   SUBROUTINE USRCEE
   PARAM NINT=5 NREAL=30
   INT VALUE-LIST=2 1
   REAL VALUE-LIST=.020 1195000.0 .01250 .330 0.0 77.10 &
      25.40 15.480 18.0 36.50 50.50 32.0 .000440 .140 &
      .8470 .1010 .10 3.0300E-09 .0000730 8314.0 3.470 &
      .001450 0.0 12100.0 1.10 59.0

CONV-OPTIONS
   PARAM CHECKSEQ=NO

STREAM-REPOR MOLEFLOW NOMASSFLOW MOLEFRAC NOMASSFRAC

REACTIONS RSCH-2 POWERLAW
   REAC-DATA 1 PHASE=V CBASIS=MOLARITY
   RATE-CON 1 PRE-EXP=2.520E+10 ACT-ENERGY=38700.0
   STOIC 1 MIXED CH3OH -1.0 / HCL -1.0 / CH3CL 1.0 / H2O &
      1.0
  POWLAW-EXP 1 MIXED CH3OH 1.0 / MIXED HCL 1.0
```

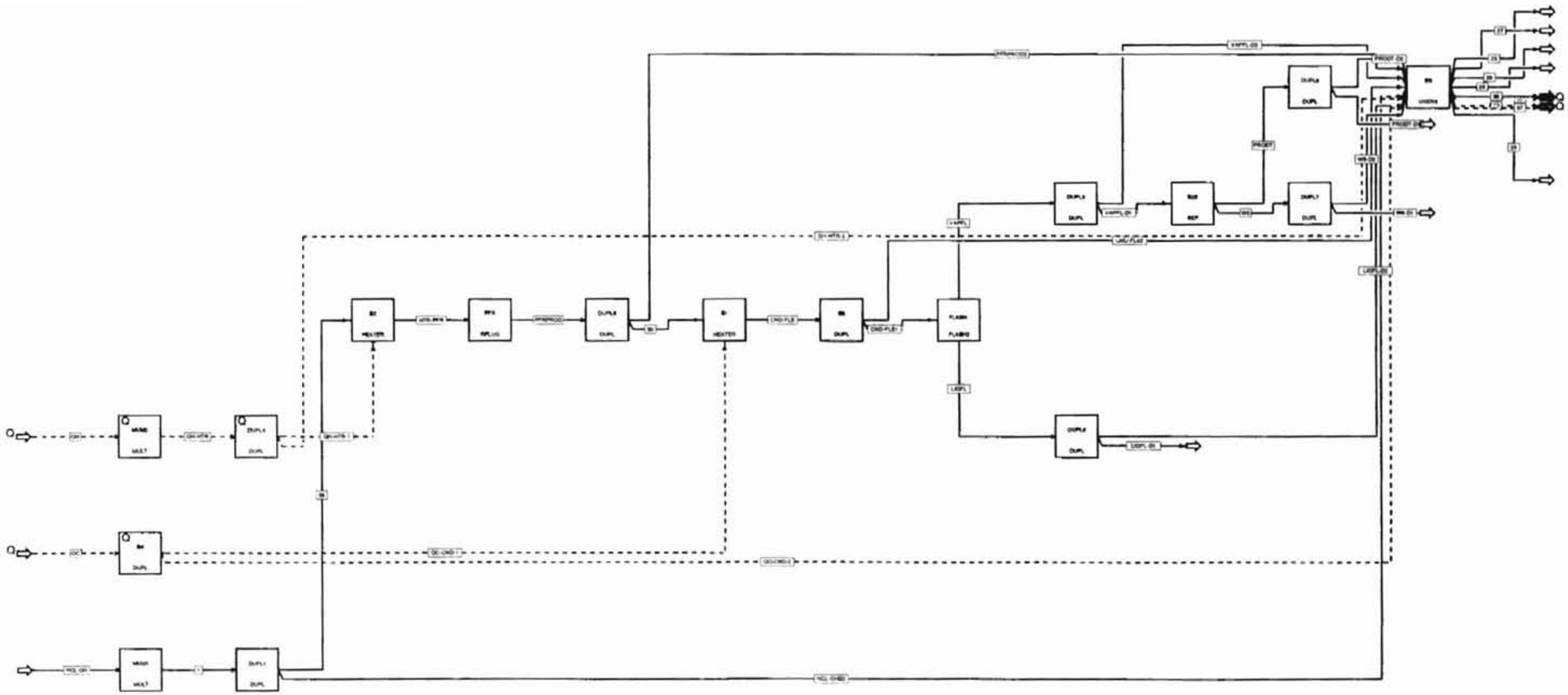


Figure D. 1 Aspen Flow Diagram for the Methyl Chloride Process

D.2 User File for Methyl Chloride Process

```
C    User Unit Operation Model (or Report) Subroutine for USER2

C  This routine has codes to evaluate all three criteria (EF, EI and C).  The routine
C  performs Singular Value Decomposition to find the singular values and hence, the
C  Condition Number of the simple methyl chloride process.  It also conducts
C   environmental impact and economic feasibility calculations.


      SUBROUTINE USRCEE (NMATI,  SIN,    NINFI,   SINFI, NMATO,
     2             SOUT,  NINFO,  SINFO,  IDSMI,  IDSII,
     3             IDSMO,  IDSIO,  NTOT,   NSUBS,  IDXSUB,
     4             ITYPE,  NINT,   INT,    NREAL,  REAL,
     5             IDS,    NPO,    NBOPST,  NIWORK, IWORK,
     6             NWORK,  WORK,   NSIZE,   SIZE,   INTSIZ,
     7             LD)
C
      IMPLICIT REAL*8 (A-H, O-Z)
C
      COMMON /USER/ RMISS,  IMISS,  NGBAL, IPASS, IRESTR,
     2           ICONVG, LMSG,   LPMSG, KFLAG, NHSTRY,
     3           NRPT,   NTRMNL, ISIZE

      DIMENSION SIN(NTOT,NMATI), SINFI(NINFI), SOUT(NTOT,NMATO),
     2        SINFO(NINFO), IDSMI(2,NMATI), IDSII(2,NINFI),
     3        IDSMO(2,NMATO), IDSIO(2,NINFO), IDXSUB(NSUBS),
     4        ITYPE(NSUBS), INT(NINT), REAL(NREAL), IDS(2,3),
     5        NBOPST(6,NPO), IWORK(NIWORK), WORK(NWORK),
     6        SIZE(NSIZE), INTSIZ(NSIZE)

C
      COMMON /NCOMP/ NCC

      DIMENSION CMV(20), CV(20), aMV(20), v(20,20), w(20), rv1(20)
      DIMENSION GKM(20,20)
      DIMENSION PHI(10),aMW(10),PHIM(10),aMF(10,10), FR(10)
C      DIMENSION CSHFLOW(20), CST(20)
      DIMENSION CST(20)

C  Opening the files in which the values of the elements of the gain matrix are
C  temporarily stored, between the manipulations of the manipulated variables
C  MV1.DAT is for storing elements of the gain matrix when CH3OH flowrate is
C  manipulated.  MV2.DAT is for storing elements of the gain matrix when the heat
C  stream 24 is manipulated.
```

```
      OPEN (UNIT=1, FILE="MV1.DAT", STATUS="OLD")
      OPEN (UNIT=2, FILE="MV2.DAT", STATUS="OLD")

C  Storing values of inlet information streams to outlet information streams

      DO 108 I = 1, NINFI
         SINFO(I) = SINFI(I)
 108  CONTINUE

C  Storing values of inlet material strams to outlet material streams

      DO 100 I = 1, NMATO
        DO 50 J=1,NTOT
          SOUT(J,I) = SIN(J,I)
 50     CONTINUE
 100  CONTINUE

      WRITE(NRPT,*)"Temperatures of SOUT streams"
      DO 101 I=1,NMATO
        WRITE(NRPT,*) I, SOUT(6,I)
 101  CONTINUE

*************************************************************************
```

```
C  Profitability Calculations
C  The following code calculates the profitability of a chemical process by using the tool,
C  annual equivalent profit (AEP).
C  AEP   = Annual Equivalent Profit:Uniform annual series of money for a
C            certain period of time.

      WRITE(NRPT,*)"Economic Feasibility"

C  Initializing aINFLOW = cash inlow into the process (costs of products)
      aINFLOW = 0.0

C  Reading cost and molecular weight (MW) values of component i from
C  the input file.
C  CST()  = Cost of each component from Chemical Market Reporter,
C           Vol 255, No. 18, 05/03/99


      DO 200 I=1,NCC
         CST(I)=REAL(I+12)
         aMW(I)=REAL(I+8)
 200  CONTINUE
```

```
C Life of project, NY, in years.
      NY = INT(2)

C Interest rate, i.
      aI = REAL(17)

C Tax Rate, TXR.
      TXR = REAL(28)

C Cost of heat supply for preheater of feed in $/J
      PREHTR  = REAL(18)
C Preheater duty, Qh
      Qh = SINFO(1)

C Cost of Cooling Water for condenser ($/s) = CWcost($/kg)*Flowrate of water(kg/s)
      CW = REAL(19)

C Calculation of the mean heat capacity of cooling water with the eqn:
C Cpmh/R = a + bTam + c/3(4Tam^2-T1T2) + d/(T1T2)
C where Tam = (T1+T2)/2

C Universal gas constant
      R = REAL(20)

C Constants in the heat capacity equation
      a = REAL(21)
      b = REAL(22)
      c = REAL(23)
      d = REAL(24)

C Inlet and outlet temperatures
      T1 =  SOUT(6,4)
      T2 =  SOUT(6,7)

      Tam = (T1+T2)/2
      Cpmh = (a + b*Tam + c/3*(4*Tam**2-T1*T2) + d/(T1*T2))*R

C Cooling water duty
      Qc = SINFO(2)

C Calculation of molar flowrate of cooling water (aNcw, in kmol) required to generate
C the heat supplied by Qc.  Calculated from eqn: Qc = Ncw*Cpmh*(T2-T1)
      aNcw = Qc/(Cpmh*(T2-T1))

C Calculation of mass flowrate, aMcw (kg/s) of cooling water.
      aMcw = aNcw*aMW(1)
```

```
C Capital Cost from Aspen Runs
      CAPCST = REAL(27)

C Working Capital = 15% of Capital Cost
      WRKCAP = 0.15*CAPCST

C Utilities cost =  sum of preheating and cooling water costs
      UTILC = Qh*PREHTR + aMcw*CW
      WRITE(NRPT,*)"UTILC=", UTILC*3600*8760

C Treatment cost per kg of organic mass
      TCPOM = REAL(25)

C Disposal cost per unit weight of the waste stream ($/kg)
      DCPWT = REAL(26)

C Cash flow for year n=0
        CSHFLOW0 = aINFLOW - CAPCST - WRKCAP

      WRITE(NRPT,*)"CAPCST=", CAPCST

C Calculation of waste disposal cost
C     Mass flowrates of waste streams to calculate waste disposal costs
          W5WT = SOUT(5,5)*SOUT(13,5)
          W6WT = SOUT(5,6)*SOUT(13,6)
C     Waste disposal cost
          DISPC = DCPWT*(W5WT+W6WT)
         WRITE(NRPT,*)"DISPC=", DISPC*3600*8760

C Calculation of waste treatment cost
C     Organic mass in waste streams to calculate waste treatment cost
          W5OM = SOUT(3,5)*aMW(3)+SOUT(4,5)*aMW(4)
          W6OM = SOUT(3,6)*aMW(3)+SOUT(4,6)*aMW(4)
C     Waste treatment cost
         TRTMNTC = TCPOM*(W5OM+W6OM)
        WRITE(NRPT,*)"TRTMNTC=", TRTMNTC*3600*8760
C Rawmaterial cost
        DO 206 J = 1, NCC
           RawMatC = RawMatC+SOUT(J,1)*aMW(J)*CST(J)
           WRITE(NRPT,*)"RawMatC=", RawMatC*3600*8760

C  Product cost.
           aINFLOW = aINFLOW+SOUT(J,2)*aMW(J)*CST(J)
           WRITE(NRPT,*)"aINFLOW=", aINFLOW*3600*8760
 206    CONTINUE
```

```
C Outflow = All costs required for the manufacture of the final product.
        OUTFLOW = RawMatC+UTILC+TRTMNTC+DISPC
        WRITE(NRPT,*)"OUTFLOW=", OUTFLOW*3600*8760

C Depreciation = (Capital Cost - Salvage Value)/Ny (Straight line depreciation method,
C               Equation 3.13)
        DEP = CAPCST/NY
        WRITE(NRPT,*)"DEP=", DEP

C Taxable income = net revenue - cash outflow - depreciation charges (Equation 3.14)
        TAXINC = (aINFLOW-OUTFLOW)*(3600*8760)-DEP
        WRITE(NRPT,*)"TAXINC=", TAXINC

 C Net income = taxable income - tax charges (Equation 3.15)
        NETINC = TAXINC*(1-TXR)
        WRITE(NRPT,*)"NETINC=", NETINC

C Cashflow = netincome + depreciation charges (Equation 3.16)
        CSHFLOW = NETINC + DEP
        WRITE(NRPT,*)"CSHFLOW=", CSHFLOW

        aNPV = CSHFLOW0
        WRITE(NRPT,*)"aNPV=",aNPV

C Net present value (Equation 3.12)
      DO 205 I = 1,NY
        aNPV = aNPV + CSHFLOW/(1+aI)**I
 205  CONTINUE
      WRITE(NRPT,*)"aNPV=", aNPV

C Annual worth factor (Equation 3.17)
      Af = (aI*(1+aI)**NY)/((1+aI)**NY-1)
      WRITE(NRPT,*)"Af=", Af

C Annual Equivalent Profit in $/yr (Equation 3.11)
      AEP = aNPV * Af
      WRITE(NRPT,65) AEP

************************************************************************

C Environmental Impact Calculations
C  E        = (Sum FR(Sum(aMFji*PHIj)))/P  (Equation 3.6) where,
C  FRi      = flowrate of waste stream i (kg/s)
C  aMFji    = mass fraction of component j in waste stream i
C  PHIj     = environmental impact index of chemical j (EIU/kg)
C  P        = total mass of product obtained (kg/s)
```

```
C  PHIM()     = Sum of products of PHI and MF of individual components in each
C                stream
C  FRPHIM() = Sum of product of FR and PHIM in each stream
C  aMW()      = Molecular weight of each component

      WRITE(NRPT,*)"Environmental Impact"
      DO 107 I=1,NMATO
        PHIM(I)=0.0
 107   CONTINUE
      FRPHIM = 0.0

      DO 110 J=1,NCC
C  Reading PHI and molecular weight (MW) values of component J from the input
C  file.
        PHI(J)=REAL(J+4)
        aMW(J)=REAL(J+8)
 110   CONTINUE

      DO 112 I=1,NMATO
       DO 111 J=1,NCC
C  Mass fraction of component J in stream I
         aMF(J,I)=(SOUT(J,I)*aMW(J))/(SOUT(5,I)*SOUT(13,I))
C  Inner loop: Sum of the product of the mass fractions and PHI of each component in
C              stream I  (From Equation 3.6)
         PHIM(I)=PHIM(I)+aMF(J,I)*PHI(J)
 111    CONTINUE

C  Calculation of flowrate of stream I.
        FR(I) = SOUT(5,I)*SOUT(13,I)
C  Outer loop:  Gives numerator of environmental impact expression (From Equation 3.6)
        FRPHIM=FRPHIM+FR(I)*PHIM(I)
        WRITE(NRPT,*)"FRPHIM=",FRPHIM
 112   CONTINUE

C  Environmental impact (E) (Equation 3.6)
      E=FRPHIM/(SOUT(3,2)*REAL(11))
      WRITE(NRPT,*)"E in EIunits/kg product"
      WRITE(NRPT,70) E

*************************************************************************
C  Controllability Analysis

C  CV()        = Deviation of Controlled Variable from its optimum value
C  MV()        = Deviation of Manipulated Variables from its optimum value
C  FEED        = Flow rate of CH3OH in the feed stream
```

```
C HEAT      = Heat supply to the flash chamber
C PROD      = Flow rate of CH3Cl in the product stream
C NV        = No. of CV or MV
C CMV()     = Ratio of CV() to MV() or elements of the gain matrix
C GKM()     = Gain Matrix
C w()       = Singular Values of the Gain Matrix
C CN        = Condition Number

      WRITE(NRPT,*)"Controllability"
C     Number of controlled (manipulated) variables or dimensions of the gain matrix.
C     Here, NV = 2. Value of INT(1) given in the input file.

      NV = INT(1)

C     Optimum values of MV and CV
      FEEDO = REAL(1)
      HEATO = REAL(2)
      PRODO = REAL(3)
      XPRDO = REAL(4)

C     Ranges of CV and MV
      FEEDR = 0.2*FEEDO
      HEATR = 0.2*HEATO
      PRODR = 0.2*PRODO
      XPRDR = 0.2*XPRDO

C Following are the expressions to calculate the physically scaled values of each
C manipulated and controlled variable (From Equation 3.4).

      CV(1) = (SOUT(3,2)-PRODO)/PRODR
      CV(2) = (SOUT(3,3)/SOUT(5,3)-XPRDO)/XPRDR
      aMV(1)= (SOUT(4,1)-FEEDO)/FEEDR

C This is the expression for the information stream supplying information about its heat
C duty to the USER block.

      aMV(2)=(SINFO(1)-HEATO)/HEATR

C Calculation of the elements of the gain matrix (GKM()). Each element is defined as
C the ratio of the physically scaled value of the controlled variable to that of the
C manipulated variable. These values are obtained by alternately commenting out the
C WRITE statements to file 1 and 2. When WRITE to file2 is commented, then MV(1)
C flowrate is manipulated and the corresponding elements of the gain matrix are
C recorded in File 1 (MV1.DAT). Then WRITE to file 1 is commented, MV(2) is
C manipulated and the corresponding elements of the gain matrix are recorded in File 2
C MV2.DAT).
```

```
      DO 10 I=1,NV
        DO 5 J=1,NV
C  Elements of the first row of the gain matrix (Equation 3.4).
        CMV(1)= CV(J)/aMV(1)
        WRITE(1, *) CMV(1)
C  Elements of the second row of the gain matrix (Equation 3.4).
        CMV(2)= CV(J)/aMV(2)
        WRITE(2, *) CMV(2)
  5     CONTINUE
        CLOSE(1)
        CLOSE(2)
 10   CONTINUE

C  Gain matrix values are read back into the Gain matrix, GKM(), from the files 1 and 2.

      DO 102 I=1,NV
        OPEN(UNIT=1, FILE="MV1.DAT",STATUS="OLD")
        READ(1,*,END=777)GKM(I,1)
 102    CONTINUE

 777    DO 103 I=1,NV
        OPEN(UNIT=2, FILE="MV2.DAT",STATUS="OLD")
        READ(2,*,END=888)GKM(I,2)
 103    CONTINUE

 30   FORMAT(5X, F16.8)

C       WRITE(NRPT,*)"Elements of the gain matrix"
      DO 105 I=1,NV
        DO 104 J=1,NV
C           WRITE(NRPT,*)GKM(I,J)
 104  CONTINUE
 105  CONTINUE


C  Singular Value Analysis to find best control strategy
C  Source:  Numerical Recipes in Fortran, 2nd Ed.
C  Control strategy being tested: FEED-PROD;HEATH-XPRD
C  This routine computes the singular value decomposition of the gain matrix as
C  GKM = U. W. V^T.


 888  n=NV
      m=NV
```

```
C House holder reduction to bidiagonal form.
    g=0.0
    scale=0.0
    anorm=0.0

    do 25 i=1,n
      l=i+1
      rv1(i)=scale*g
      g=0.0
      s=0.0
      scale=0.0
      if(i.le.m)then
        do 11 k=i,m
          scale=scale+abs(GKM(k,i))
11      continue
        if(scale.ne.0.0)then
          do 12 k=i,m
            GKM(k,i)=GKM(k,i)/scale
            s=s+GKM(k,i)*GKM(k,i)
12        continue
          f=GKM(i,i)
          g=-sign(sqrt(s),f)
          h=f*g-s
          GKM(i,i)=f-g
          do 15 j=l,n
            s=0.0
            do 13 k=i,m
              s=s+GKM(k,i)*GKM(k,j)
13          continue
            f=s/h
            do 14 k=i,m
              GKM(k,j)=GKM(k,j)+f*GKM(k,i)
14          continue
15        continue
          do 16 k=i,m
            GKM(k,i)=scale*GKM(k,i)
16        continue
        endif
      endif
      w(i)=scale *g
      g=0.0
      s=0.0
      scale=0.0
      if((i.le.m).and.(i.ne.n))then
        do 17 k=l,n
```

```
         scale=scale+abs(GKM(i,k))
 17     continue
       if(scale.ne.0.0)then
        do 18 k=l,n
          GKM(i,k)=GKM(i,k)/scale
          s=s+GKM(i,k)*GKM(i,k)
 18      continue
        f=GKM(i,l)
        g=-sign(sqrt(s),f)
        h=f*g-s
        GKM(i,l)=f-g
        do 19 k=l,n
          rv1(k)=GKM(i,k)/h
 19      continue
        do 23 j=l,m
          s=0.0
          do 21 k=l,n
            s=s+GKM(j,k)*GKM(i,k)
 21        continue
          do 22 k=l,n
            GKM(j,k)=GKM(j,k)+s*rv1(k)
 22        continue
 23      continue
        do 24 k=l,n
          GKM(i,k)=scale*GKM(i,k)
 24      continue
       endif
      endif
      anorm=max(anorm,(abs(w(i))+abs(rv1(i))))
 25  continue

C  Accumulation of right hand transformations
    do 32 i=n,1,-1
      if(i.lt.n)then
       if(g.ne.0.0)then

C  Double division to avoid possible underflow
        do 26 j=l,n
          v(j,i)=(GKM(i,j)/GKM(i,l))/g
 26      continue
        do 29 j=l,n
          s=0.0
          do 27 k=l,n
            s=s+GKM(i,k)*v(k,j)
 27        continue
          do 28 k=l,n
```

```
            v(k,j)=v(k,j)+s*v(k,i)
28          continue
29        continue
        endif
        do 31 j=l,n
          v(i,j)=0.0
          v(j,i)=0.0
31      continue
      endif
      v(i,i)=1.0
      g=rv1(i)
      l=i
32  continue

C  Accumulation of left hand transformations
    do 39 i=min(m,n),1,-1
      l=i+1
      g=w(i)
      do 33 j=l,n
        GKM(i,j)=0.0
33    continue
      if(g.ne.0.0)then
        g=1.0/g
        do 36 j=l,n
          s=0.0
          do 34 k=l,m
            s=s+GKM(k,i)*GKM(k,j)
34        continue
          f=(s/GKM(i,i))*g
          do 35 k=i,m
            GKM(k,j)=GKM(k,j)+f*GKM(k,i)
35        continue
36      continue
        do 37 j=i,m
          GKM(j,i)=GKM(j,i)*g
37      continue
      else
        do 38 j= i,m
          GKM(j,i)=0.0
38      continue
      endif
      GKM(i,i)=GKM(i,i)+1.0
39  continue

C  Diagonalization of the bidiagonal form:  Loop over singular values, and over allowed
C  iterations.
```

```
      do 49 k=n,1,-1
        do 48 its=1,30

C  Test for splitting
          do 41 l=k,1,-1
            nm=l-1
            if((abs(rv1(l))+anorm).eq.anorm)  goto 2
            if((abs(w(nm))+anorm).eq.anorm)  goto 1
 41         continue

C  Cancellation of rv1(l), if l>1.
  1        c=0.0
          s=1.0
          do 43 i=l,k
            f=s*rv1(i)
            rv1(i)=c*rv1(i)
            if((abs(f)+anorm).eq.anorm) goto 2
              g=w(i)
              h=DSQRT(DABS(f**2)+DABS(g**2))
              w(i)=h
              h=1.0/h
              c= (g*h)
              s=-(f*h)
              do 42 j=1,m
                y=GKM(j,nm)
                z=GKM(j,i)
                GKM(j,nm)=(y*c)+(z*s)
                GKM(j,i)=-(y*s)+(z*c)
 42             continue
 43         continue
  2        z=w(k)

C  convergence
          if(l.eq.k)then

C  Singular value is made nonnegative.
            if(z.lt.0.0)then
              w(k)=-z
              do 44 j=1,n
                v(j,k)=-v(j,k)
 44             continue
            endif
            goto 3
          endif
          if(its.eq.30) pause 'no convergence in svdcmp'
```

```
C Shift from bottom 2-by-2 minor.
        x=w(l)
        nm=k-1
        y=w(nm)
        g=rv1(nm)
        h=rv1(k)
        f=((y-z)*(y+z)+(g-h)*(g+h))/(2.0*h*y)
        g=DSQRT(DABS(f**2)+1.0)
        f=((x-z)*(x+z)+h*((y/(f+sign(g,f)))-h))/x

C Next QR transformation.
        c=1.0
        s=1.0
        do 47 j=l,nm
          i=j+1
          g=rv1(i)
          y=w(i)
          h=s*g
          g=c*g

C Pythagoros function
          z=DSQRT(DABS(f**2)+DABS(h**2))
          rv1(j)=z
          c=f/z
          s=h/z
          f= (x*c)+(g*s)
          g=-(x*s)+(g*c)
          h=y*s
          y=y*c
          do 45 jj=1,n
            x=v(jj,j)
            z=v(jj,i)
            v(jj,j)= (x*c)+(z*s)
            v(jj,i)=-(x*s)+(z*c)
 45         continue
          z=DSQRT(DABS(f**2)+DABS(h**2))

C Rotation can be arbitraryif z = 0.
          w(j)=z
          if(z.ne.0.0)then
            z=1.0/z
            c=f*z
            s=h*z
          endif
          f= (c*g)+(s*y)
          x=-(s*g)+(c*y)
```

```
          do 46 jj=1,m
            y=GKM(jj,j)
            z=GKM(jj,i)
            GKM(jj,j)= (y*c)+(z*s)
            GKM(jj,i)=-(y*s)+(z*c)
 46       continue
 47     continue
        rv1(l)=0.0
        rv1(k)=f
        w(k)=x
 48   continue
  3    continue
 49  continue
```

C Printing values of the U (Left Singular Vector) array.

```
    WRITE(NRPT,*)"Elements of U"
    DO 56 I=1,m
      DO 51 j=1,n
        WRITE(NRPT,60)GKM(i,j)
 51    CONTINUE
 56  CONTINUE
```

C Printing values of V (Right Singular Vector) array.

```
    WRITE(NRPT,*)"Elements of V"
    DO 57 i=1,m
      DO 53 j=1,n
        WRITE(NRPT,60)v(i,j)
 53    CONTINUE
 57  CONTINUE


    WRITE(NRPT,*)"Singular Values of the Gain Matrix"
    DO 52 i=1,n
      WRITE(NRPT,55)w(i)
 52  CONTINUE

    do 503 j=2,n
      a=w(j)
      DO 500 i=j-1,1,-1
        if(w(i).le.a)goto 502
        w(i+1)=w(i)
500    CONTINUE
      i=0
502    w(i+1)=a
```

```
 503  continue

     WRITE(NRPT,*)"Sorted array of singular values"
     DO 504 i=1,n
       WRITE(NRPT,*)w(i)
 504  CONTINUE

C  Calculation of the condition number.  It is the ratio of the max (singular
C  value) to the min (singular value) (Equation 3.5).

     CN=w(N)/w(1)
     WRITE(NRPT,*)"CONDITION NUMBER"
     WRITE(NRPT,*)CN

  55  FORMAT(F8.3)
  60  FORMAT(F10.6)
  65  FORMAT(F20.4)
  70  FORMAT(F10.3)

 999  RETURN
     END
```

APPENDIX E

FLEXIBILITY, RESILIENCY AND SAFETY

E.1 Flexibility

Swaney and Grossmann (1985a) suggested a flexibility index to measure the flexibility of a chemical process. The main idea is to measure the size of the region of feasible steady state operation in the space of uncertain parameters, θ (eg., changes in process parameters, such as heat transfer coefficients as well as disturbances). This method has already been discussed briefly in Chapter 2 . The concept is better illustrated by Figure E.1.

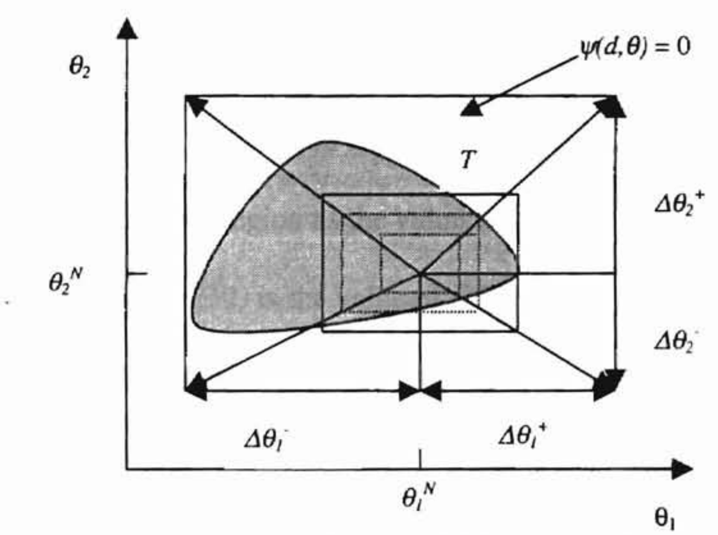


Figure E. 1 Flexibility Analysis

Constraints on a general plant are represented by the following equality and inequality expressions:

$$h(d,m,x,\theta)=0 \quad \text{E. 1}$$

$$g(d,m,x,\theta)\le 0 \quad \text{E. 2}$$

where, *d*= design variables

m=manipulated variables

x=state variables

θ=uncertain parameters

Since $x=x(m)$, function reduces to,

$$f(d,m,\theta) \leq 0 \qquad \text{E. 3}$$

which gives the feasible operating region for the plant. This is represented by the shaded region, $\psi(d,\theta) = 0$, in Figure E.1 .

θ varies as : $\theta^- <= \theta <= \theta^+$

θ^N = Nominal value of θ

δ = max. change in θ (same amount assumed in both positive and negative directions).

The independent parameters, $\theta 1$ and $\theta 2$, are characterized by normal distributions, which gives rise to a joint distribution whose contours are the hyperrectangles. They are inscribed within the feasible region as the value of δ increases as shown in Figure E.1. Now, the flexibility index *(FI)* is the value of δ that gives maximum inscribed hyperrectangle area within the feasible operating region. Alternative designs are compared with *FI*, the larger the value of *FI*, the more flexible is the design.

Straub and Grossmann (1990) extended the flexibility index (*FI*) described above to develop a quantitative measure called expected stochastic flexibility, *E(SF)*, for the flexibility of a design to withstand uncertainties in the continuous parameters and discrete states. Uncertainties in the continuous parameters are changes in flowrates, temperatures etc, and uncertainties in discrete parameters are the availability/unavailability of pieces of equipment. The stochastic flexibility (*SF*) is the cumulative probability of the joint distribution, represented by the hyperrectangles in Figure E.1 that lies within the feasible region. Thus, mathematically SF is the integral of the joint distribution over the shaded region.

The discrete uncertainty involves changes in the state of a design which result in different feasible regions. This is shown in Figure E.2. Normal operation is represented by state 1 and state 2 represents the process which experienced a failure in the functioning of some equipment, and hence the capacity is reduced.

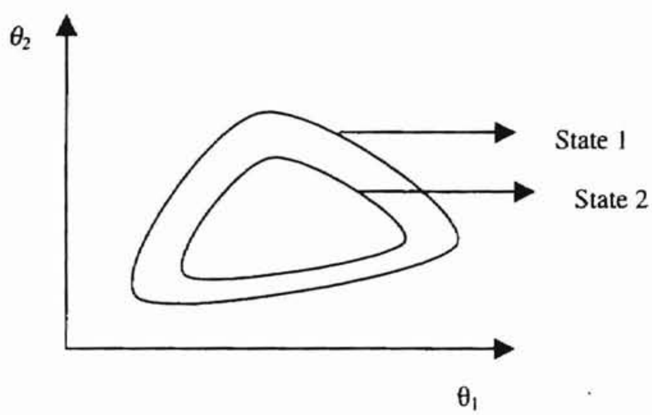


Figure E. 2 Effect of Discrete Uncertainty on the Feasible Region

The expected stochastic flexibility, $E(SF)$, is calculated by summing up the products of the probability for each discrete state and its corresponding SF.

Now, in addition to the equations given by E.1 and E.2, the system is repesented by capacity constraints given by:

$$j(d,m,x,\theta) \leq Dy \qquad \text{E. 4}$$

Where, D = diagonal matrix of L design variables (d_l, l=1,...L) that define the capacity of units, and y = vector of Boolean variables defining the availability of the L pieces of equipment.

When a discrete uncertainty is active $y_l = 1$ and when inactive $y_l = 0$. Each y_l is associated with a probability of P, where $P\{y_l = 1\} = p_l$ and $P\{y_l = 0\} = 1\text{-}p_l$. The probability of being in an active state is given by:

$$P_l = \frac{\mu}{\lambda + \mu} \qquad \text{E. 5}$$

where, λ = failure rate and μ = repair rate of equipment. The boolean variables give rise to different system states and an associated state probability. Each state, S_i, represents a different combination of the 0-1 values for the vector y. The state probability is defined as follows:

$$P(S_i) = \prod_{l \in Y_1^i} p_l \prod_{l \in Y_0^i} (1 - p_l) \quad i = 1, \ldots 2^L \qquad \text{E. 6}$$

where, $Y_0^i = \left\{ l \mid y_l^i = 0 \right\}$ and $Y_1^i = \left\{ l \mid y_l^i = 1 \right\}$.

Now, the stochastic flexibility of the system for a given state, S_i, can be calculated by integrating the distribution function over the feasible region. SF is given by:

$$SF(S_i) = \int_{\theta : \psi(d^i, \theta)} j(\theta) d\theta \qquad \text{E. 7}$$

where, $\psi(d^i, \theta) \leq 0$ is the feasible operating region, and $j(\theta)$ is the joint distribution of the continuous uncertainties.

Expected stochastic probability, $E(SF)$, is given by:

$$E(SF) = \sum_{i=1}^{2^L} SF(S_i) \times P(S_i) \qquad \text{E. 8}$$

$E(SF)$ represents the average stochastic flexibility that is measured over a long period of time.

E.2 Resiliency

Lewin (1996) describes resiliency as the degree to which the control objectives can maintain the outputs of the multivariable process at the required setpoints despite uncontrollable external disturbances and uncertainties in the process model. A simple graphical method, the Disturbance Cost, was developed. This helped in the diagnosis of this disturbance resiliency for processes affected by disturbance vectors.

Effect of control variables, CV, and disturbances, DV, on the process output, y, can be described by the equation:

$$Y(s) = P(s)CV(s) + P_d(s)DV(s) \qquad \text{E. 9}$$

From this model, a complete disturbance rejection is possible when

$$CV(s) = -P^{-1}(s)DV', \qquad \text{E. 10}$$

where,

$$DV'(s) = Pd(s)DV(s) \qquad \text{E. 11}$$

A quantitative measure of the effort required to reject a given disturbance vector is the Euclidean norm:

$$|CV|_2 = |P^{-1}P_dDV|_2 \qquad \text{E. 12}$$

The measure, $|CV|_2$ is called the disturbance cost (Lewin, 1996). This is a measure of the costs involved in the feed back effort required to reject the vector d(s). An alternative, normalized, measure of the effect of disturbance direction of performance is the disturbance condition number (*DCN*). *DCN* is given by:

$$\frac{|CV|_2}{|DV'|_2} = \frac{|P^{-1}(s)DV'(s)|_2}{|DV'(s)|_2} \qquad \text{E. 13}$$

The plant disturbance condition number is given by:

$$\kappa_d(P) = \frac{|P^{-1}(s)DV'(s)|_2}{|DV'(s)|_2}\sigma(P) \qquad \text{E. 14}$$

The disturbance condition number lies between 1.0 and the plant condition number.

Thus, either the disturbance cost (*DC*) or the disturbance condition number can be used to measure the resiliency of the process.

E.3 Safety

The concept of 'inherent safety' has been popular for a long time, but despite its benefits related to safety, health and environment (SHE), as well as to costs there have been few recognized examples of its application to chemical plant design (Mansfield, 1996). Mansfield in his article points out the benefits of implementing the principles of inherent safety and suggested strategies to achieve it too. Checking a process against these principles, though is a good measure, is very subjective, hence a semi quantitative measure has been developed by the Dow Chemical Co. called the Fire and Explosion Index (*F&EI*) (Gowland, 1996). The *F&EI* provides a comparative measure of the overall risk of fire and explosion of a process. In determining the *F&EI* for a given process unit, the engineer assigns numerical penalties for specific hazards. The procedure for calculating the F&EI is given in Figure E.3. The definitions of the terms used in the flowsheet are:

MF = Material factor: It is derived from the intrinsic rates of potential energy release from fire or explosion caused by combustion or chemical reaction.

F_1 = General process hazards factor: Hazards due to exothermic and endothermic chemical reactions, material handling, indoor process units etc come under this category (For more details refer to the article by Gowland (1996)).

F_2 = Special process hazards factor: Hazards due to toxic materials, sub atmospheric pressures, operation at or near flammable range, dust explosion etc come under this category.

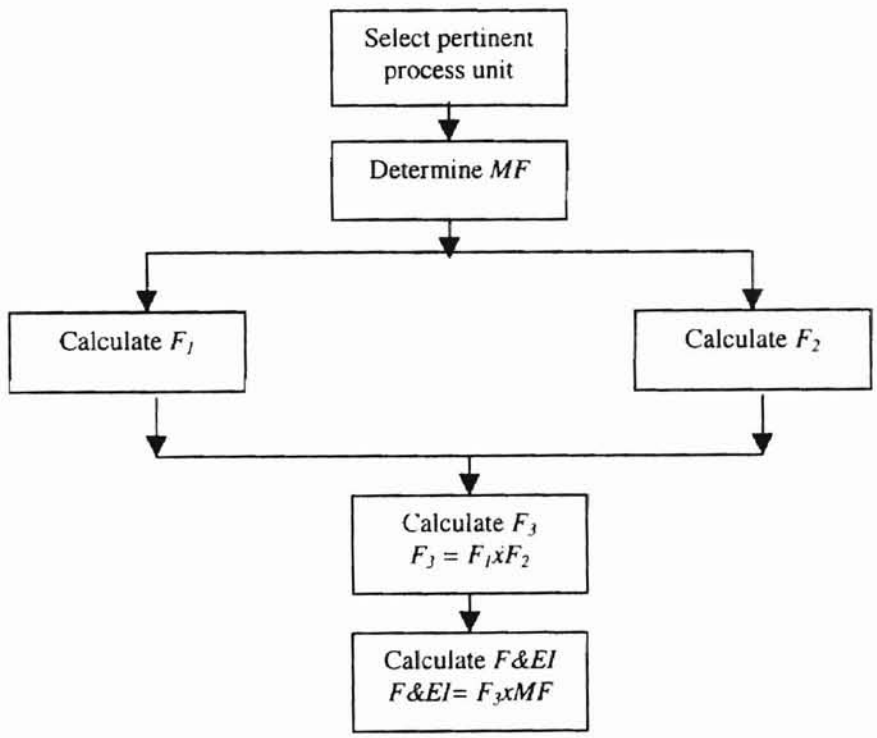


Figure E. 3 Flowsheet for Calculating Fire & Explosion Index

APPENDIX F

MULTI-CRITERIA DECISION MAKING

F.1 Introduction

A common practice in industry is to analyze complex problems and make decisions based on multiple criteria. The current research work also involves making a decision in choosing the best design from a set of alternatives with respect to multiple criteria as listed in the Section 3.1.2. The set of potential outcomes or alternatives from which to choose are the essence of decision making (Saaty, 1994). As there is never an exact solution for a problem of choosing between alternatives, the final solution is always a compromise between the various criteria. The following sections discuss two popular tools for multi-criteria decision making, the analytic hierarchy process and (AHP) and multi-objective optimization.

F.2 Analytic Hierarchy Process (AHP)

Analytic hierarchy process is a multi criteria decision making tool, first founded by Dr. Thomas Saaty and Dr. Ernest Forman, co-founders of Expert Choice, Inc. AHP has successfully been used in the US embassy to choose an email system for embassies. Also, Toronto Hydro used Expert Choice software to rank over 800 job applicants for human resources (Saaty, 1999).

Analytic Hierarchy Process (AHP) breaks a problem down and then aggregates the solutions of all the subproblems into a conclusion (Saaty, 1994). AHP facilitates decision making by organizing perceptions, feelings, judgements and memories into a framework that exhibits the forces that influence a decision. For a multiple criteria decision making problem of the form (Bryson and Mobolurin, 1994):

$$Max\left\{[Z_{i1},....,Z_{iN}]^T \mid i \in I\right\} \qquad \text{F. 1}$$

where, i is the index set of M alternatives; j is the index set of N criteria; and Z_{ij} is the score (a positive number) for alternative i with respect to the j-th criterion. A popular approach to solving the problem given in Equation F.1 is to formulate the function as an equivalent weighing problem of the form (Bryson and Mobolurin, 1994):

$$Max\left\{\sum_j w_{f,j} Z_{ij} \mid i \in I; \sum_j w_{f,j} = 1; w_{f,j} \geq 0\right\} \qquad \text{F. 2}$$

The necessary condition for the existence of this function is that the criteria be preferentially independent. The major problem with formulating the problem in F. 1 as F. 2 is choosing the weighing factors. The weighing factors should be a reflection of the decision maker's beliefs in the relative importance of each of the criteria. AHP is a useful technique in capturing relevant weighing information from the decision maker (through verbal, numerical or graphical means) without requiring an exorbitant commitment of time (Bryson and Mobolurin, 1994).

Weights to AHP are determined using pairwise comparison between each pair of criteria (Bryson and Mobolurin, 1994). Pairwise comparisons are then transformed to a numerical value. The result is a positive reciprocal matrix $A = \{a_{jk}\}$ with $a_{kj}=1/a_{jk}$, where a_{jk} is the numerical equivalent of the comparison between criteria j and k. The normalized weight vector, w_f, is obtained by solving the equation,

$$Aw = e_{Max} w_f \qquad \text{F. 3}$$

where e_{Max} is the largest eigenvalue and w is a normalized eigenvector associated with A and e_{Max}. Once the weighting factors are calculated with Equation F.3, Equation F.2 can be used to maximize the objective of the problem.

F.3 Multi-Objective Optimization (MOO)

Another popular tool for multiple criteria decision making is multi-objective optimization. This tool is generally used for solving problems formulated as follows:

Maximize or Minimize $MO_1 = f(x,y), MO_2 = f(x,y), \ldots\ldots, MO_3 = f(x,y)$ F. 4

subject to $g(x,y) = 0$ and

$h(x,y) \geq 0$

In those multi-objective optimization problems where, the decision maker articulates his preferences in advance of the analysis, there are two popular approaches to solve the problem: goal programming and compromise programming. Goal programming is used when the decision maker gives a specific goal to be achieved for each objective (Dantus, 1999). Then, the solution, which is closest to all the goals is chosen as the optimum point.

The other approach, compromise programming, differs from goal programming in that it tries to find a solution, which is close to an ideal point as opposed to finding a solution close to a specific goal (Dantus, 1999). Generally, the ideal solution is not feasible, but it can be used to find the best compromise solution when there are a lot of objectives to achieve. Thus, the compromise solution is defined as x_j^* such that

$$Min\ \ L_j(x) = L_j(x_j^*) \qquad \text{F. 5}$$

where, Lj = distance from the ideal point, and is defined as:

$$L_j = \sum_{i=1}^{n} w_i^j (z_i^* - z_i(x))^j \qquad \text{F. 6}$$

where, w = preference weight

j = compromise index, where $1 \leq j \leq \infty$.

A recent method by which multi-objective problems are being solved and which is gaining popularity is to generate a pareto set with a multiobjective genetic algorithm. Balling (Balling, 1999) used this approach along with the city and state officials to solve a city planning problem with multiple competing objectives. The city planning problem comprised of developing future land use and transportation plans for a particular region. There were about 9 competing objectives like, traffic congestion, housing etc. Their approach was to generate a set of plans called the Pareto set, which is a set in which no single alternative has been found to be better than the other. A multi objective genetic algorithm is used to generate the Pareto set. Then, the pareto set is scanned by the decision-maker with a graphical tool (the pareto set scanner) that they developed to find the optimum solution.

This approach can be applied to the current problem as shown in Figure F.1. This approach demands an intensive coordinated effort of all the departments in the industry involved in making a decision. All the departments need to work together to come with a list of all possible alternatives to the existing design structure. The current research seeks to override the "green chemistry" concept of improving the chemistry of process alternatives to make them more environmental friendly and choosing the best out of the alternatives. This research incorporates operability factors also in evaluating and comparing process alternatives. Thus, the objectives for the current research are to maximize profitability ($\$$), minimize environmental impact (E) and maximize operability (O). The multiobjective optimization problem can be formulated as (See Figure F.1):

$$\begin{gathered} \text{Max}\ (\$) \\ \text{Min}\ (E) \end{gathered} \qquad \text{F. 7}$$

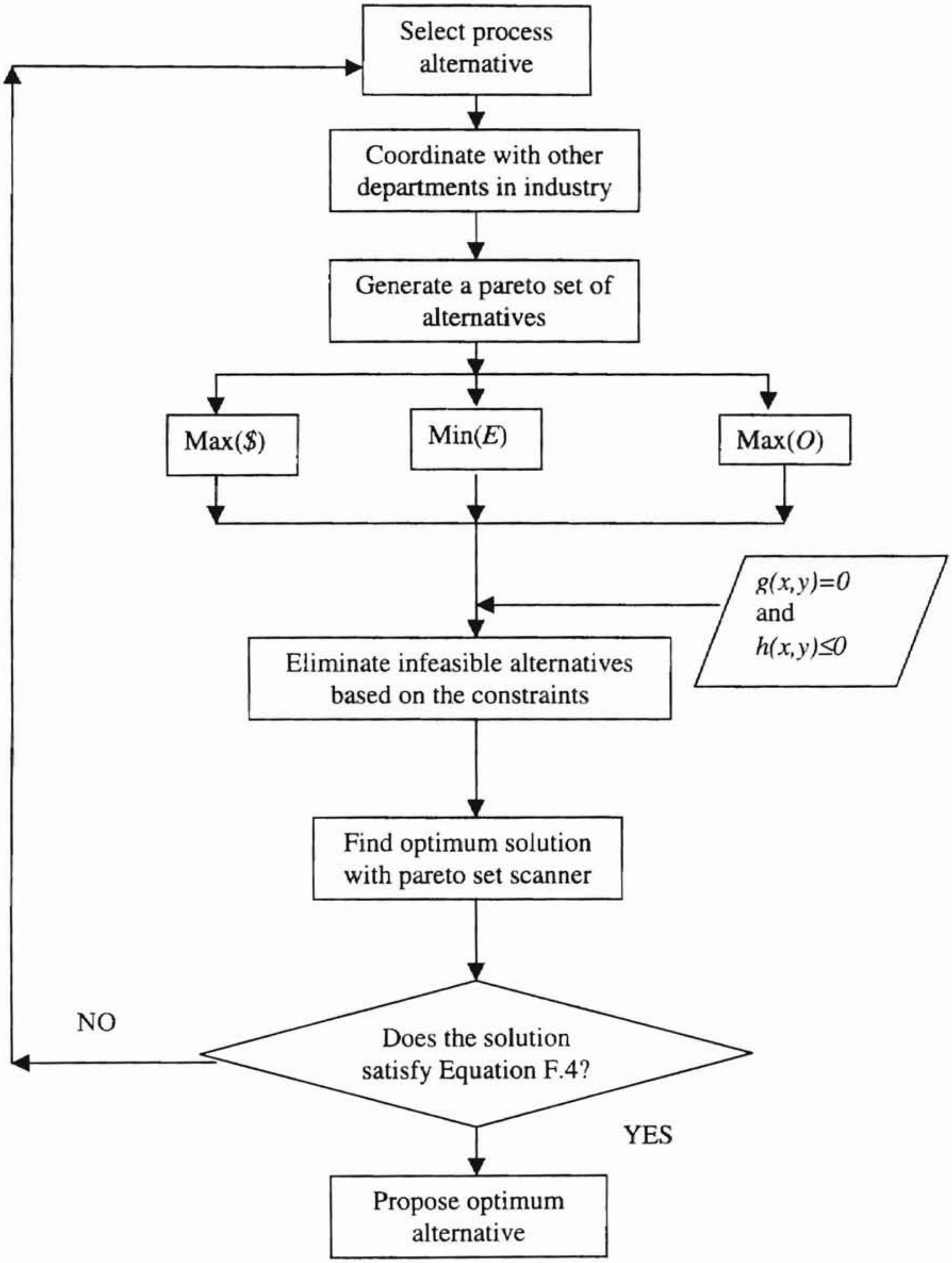


Figure F. 1 Multi-Objective Genetic Algorithm for Comparing Alternative Process Designs

$$\text{Max}\ (O)$$

subject to,

$$g(x,y) = 0 \text{ and}$$

$$h(x,y) \geq 0$$

The constraints allow the elimination of infeasible alternatives right away, which in Balling's problem eliminated millions of plans (Balling, 1999). The pareto set scanner when developed for the current problem appears as follows.

The current design of the chemical process appears on the screen. Three slider bars are used to represent the three objectives given in Equation F.7. As the user moves each slider bar with the mouse, the relative importance of the corresponding objective is increased or decreased. The tool automatically identifies the alternative design, which is optimal for the mix of relative importance indicated by the position of the slider bars from the pareto set, and displays this alternative on the screen. This tool allows the decision maker to rapidly scan through the numerous alternatives that the engineers can come up with and find that which best satisfies them.

Finally, Balling (1999) says that the reason why optimization is not used to the fullest extent in industry is probably because industry didn't have good experiences with optimization. This failure in utilization of optimization techniques is due to an improper formulation of the optimization problem. The difficulty in formulation of the optimization problem is because people are generally not very clear as to what exactly they want, until they see the various probabilities. For this reason, the tool that Balling developed (which covers all possible alternatives) is an effective way to solve a multi-objective optimization problem to obtain an optimum solution that satisfies the user.

VITA

USHA GOLLAPALLI

Candidate for the Degree of

Master of Science

Thesis: FEASIBILITY AND OPERABILITY ANALYSIS OF CHEMICAL PROCESS ALTERNATIVES

Major Field: Chemical Engineering

Biographical:

Personal Data: Born in Hyderabad, India, On April 22, 1976, the daughter of Sarma and Lakshmi Gollapalli.

Education: Graduated from Visakha Valley School, Visakhapatnam, India in May 1993; received a Bachelor of Technology degree in Chemical Engineering from Andhra University, Visakhapatnam, India in July 1997. Completed the requirements for the Master of Science degree with a major in Chemical Engineering at Oklahoma State University in December 1999.

Experience: Employed by Oklahoma State University as a Teaching Assistant from August 1997 to July 1998. Worked for Food and Agricultural Products Research Technology Center for the Summer of 1998. Employed by Oklahoma State University again as a Research Assistant from August 1998 to August 1999.

Professional Memberships: American Institute of Chemical Engineers.