THE INTEGRATION OF DOW'S FIRE AND EXPLOSION INDEX

INTO PROCESS DESIGN AND OPTIMIZATION

TO ACHIEVE AN INHERENTLY SAFER DESIGN

A Thesis

by

JAFFEE SUARDIN

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

August 2005

Major Subject: Chemical Engineering

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Approved by:

Chair of Committee,   M Sam Mannan
Committee Members, Mahmoud El-Halwagi
                          David Blackwell
Head of Department, Kenneth R Hall

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ABSTRACT

The Integration of Dow's Fire and Explosion Index into Process Design and

Optimization to Achieve an Inherently Safer Design. (August 2005)

Jaffee Suardin, B.S., Bandung Institute of Teknologi, Indonesia

Chair of Advisory Committee: Dr Sam Mannan

The integration of the safety parameter into process design and optimization is essential. However, there is no previous work in integrating the fire and explosion index (F&EI) into design and optimization. This research proposed a procedure for integrating safety into the design and optimization framework by using the safety parameter as optimization constraint. The method used in this research is Dow's Fire and Explosion Index which is usually calculated manually.

This research automates the calculation of F&EI. The ability to calculate the F&EI, to determine loss control credit factors and business interruption, and to perform process unit risk analysis are unique features of this F&EI program. In addition to F&EI calculation, the F&EI program provides descriptions of each item of the penalties, chemicals/materials databases, the flexibility to submit known chemical/material data to databases, and material factor calculations. Moreover, the sensitivity analyses are automated by generating charts and expressions of F&EI as a function of material inventory and pressure. The expression will be the focal point in the process of integrating F&EI into process design and optimization framework.

The proposed procedure of integrating F&EI into process design and optimization framework is verified by applying it into reactor-distillation column system. The final result is the optimum economic and inherently safer design for the reactor and distillation column system.

DEDICATION

To Allah SWT for His endless blessing

To Mama for the continuous love, warmness and comfortness

To Daddy for the love, supports, critiques, encouragement and inspiration by being the best chemical engineer I've ever seen.

To my sisters Uni Nadia and Lucille who have showered me with sweet and caring love.

To Anis for her love, patience, and never-ending motivation.

To safety society for their continuous efforts in finding "safety"

"take to learning as far as possible, but ALLAH SWT will not give its rewards until you translate it into action"

(Mohammad SAW)

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I would like to express thanks to Dr. El-Halwagi for his kindness and his knowledge in process optimization that has guided me throughout the research and during my study in pursuing my master's degree. I also am grateful to Dr. Blackwell for giving me ideas about economic matter. As we know, economics is really important in performing process optimization.

I also thank Dr. Wang for reviewing my ideas and thesis, Zuher Syihab for guiding me in computer programming and Tanya Mohan for her knowledge in using LINGO.

I thank Mike O'Connor for his endless support to the Mary Kay O'Connor Process Safety Center to become the leading university institution in process safety. I also acknowledge and thank Dr. West, Dr. Keren, and all group members and staff at the Mary Kay O'Connor Process Safety Center for their support and critiques. I also would like to express thanks to Towanna Hubacek, Ninette Portales, Donna Startz and Mary Cass for helping me with all the paperwork during my master's program.

Thanks to all my friends and colleagues for making this such a good experience and making this city feel like home. I realize that many people contributed to my studies, and I thank them all.

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CHAPTER I

INTRODUCTION

1.1. OVERVIEW

Along with its advances and benefits to the society, the chemical industry has also brought along the hazards that need to be managed appropriately. Unfortunately in some occurrences, lack of knowledge, technology, or failures in management systems has led to tragic incidents. Examples are the Flixborough incident with 28 fatalities (Crowl & Louvar, 2001), the Bhopal incident with more than 2,000 fatalities (Crowl & Louvar, 2001), the Pasadena-Texas explosion with 23 fatalities (Crowl & Louvar, 2001), and the more recent Texas City-refinery explosion which cost the lives of 15 people, not to mention multiple injuries, capital loss, lawsuits, decreased stock price, ruined image/brand, etc. Loss prevention, as the term used by insurance industry, comes not only from the cost of replacing the damaged plant or equipment and third party claim but also from the loss of revenue from the opportunity of production and sales.

"What exactly had happened?" and "what are the reasons behind those incidents?" are the questions that can be raised. In answering those questions, we need to understand what the hazards are. Adapted from the Center for Chemical Process Safety (CCPS), hazard is defined as physical or chemical characteristic that has the potential for causing harm to people, the environment, or property (Crowl, 1996). It is very important

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This thesis follows the style and format of the *Journal of Loss Prevention in the Process Industries.*

to note that the hazards are intrinsic and are the basic properties of the material or its conditions of use. For example, 10,000 lbs of propane holds the same amount of energy which could be released by 28 tons of TNT. Those energies are inherent to the propane, cannot be changed, and will be released when equipment or other failure happens and leads to an incident.

While an "inherently safe" plant infers a plant that has no hazards on an absolute basis, such plant with "zero risk" might be impossible to design and to operate. Therefore, the need to manage hazards and risks strategically and systematically arises and one of the strategies is inherently safer design concept (as opposed to inherently safe plant). In addition, the best strategy seeks to combine inherently safer design with process design and optimization at the early stages of design where the degree of freedom for modification is still high.

In the next sections, the objectives, the details of inherently safer design concept, pertinent previous research, process design and optimization, and their current industry practice are discussed. The description of the methodology, design and optimization models, and summary of the research are presented as well.

1.2 INHERENTLY SAFER DESIGN

While layers of protection assist in controlling and managing risks associated with the hazards, it is better to reduce the inherent hazard. The term "Inherently Safer Design" started appearing in safety discussion after Trevor Kletz introduced this concept

as an identifiable element of process safety in one of his most famous phrases "What You Don't Have Can't Leak".

Inherently safer design infers the elimination of hazards as much as possible out of a chemical or physical process permanently as opposed to using layers of protection. It is a challenge for engineers to design an optimal and inherently safer process to produce good quality and high yield products within acceptable economic limits. There are four primary principles of inherently safer design concept proposed by Kletz (1991):

1. Intensification – to reduce the inventories of hazardous materials as more inventory of hazardous chemicals mean more hazards.

2. Substitution – to use less hazardous materials in the process.

3. Attenuation – to operate a process at less dangerous process conditions (pressure, temperature, flow rate, etc).

4. Limitation of effects – to design the process according to the hazards offered by the process in order to reduce the effects of the hazards.

In the US, inherently safer design started receiving more attention following a highly-praised paper presented by Kletz in 1985 at the 19th Loss Prevention Symposium of the American Institute of Chemical Engineers (AIChE) (Hendershot, 1999).

1.3 SAFETY STUDIES

In the recent years, public concern about safety issues has increased due to risk posed by more complex and more extreme conditions of the chemical industries to the employees, communities living near the site, properties, and environment. In the

Chemical Process Industries (CPI) point of view, there are also potential economic and business losses. Therefore, CPI has had significant efforts to manage and to control the hazards. The most common and traditional approach has focused on layers of protection (LOP) where additional safety devices and features are added to the process, as shown in Figure 1.2.

The LOP method has been successful in producing an excellent safety record. However, this approach has several disadvantages as listed below (Crowl 1996):

- LOP increase the complexity of the process, and hence the capital and operating cost. In the oil and gas industries, 15-30 % of the capital cost goes to safety issues and pollution prevention (Palaniappan & Srinivasan, 2004).

- The hazards within the process remain, even when LOP are installed and are built based on the anticipation of incidents, as shown in Figure 1.2 (a). Since nature might find creative ways to release hazards, there are always dangers from unanticipated failure mechanisms that the LOP are not ready for, as shown in Figure 1.2 (b).

- Since no LOP can be perfect, failures or degradation in LOP may pose risks offered by the hazards that lead to incidents, as shown in Figure 1.2 (c).

Other efforts by the industries and researchers toward safety studies tend to focus on hazard identification and control. There has been some work in developing more advanced hazard and risk analysis methods such as Failure Modes and Effects Analysis (FMEA), Fault Tree Analysis (FTA), Event Tree Analysis (ETA), Cause-Consequences Analysis (CCA), Preliminary Hazard Analysis, Human Reliability Analysis (HRA) and
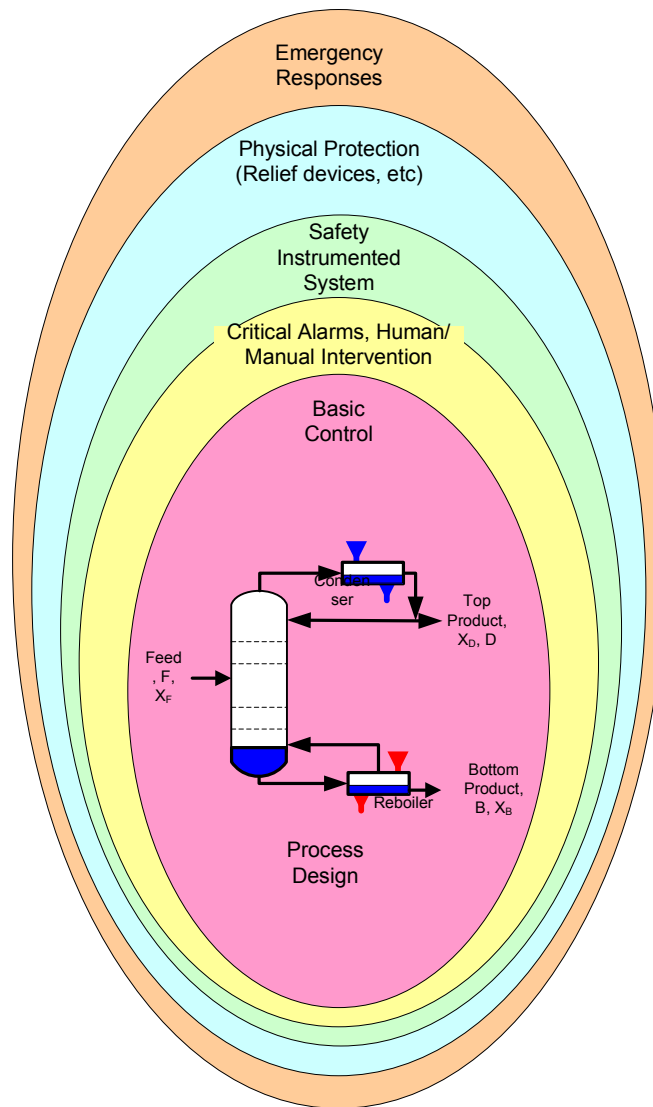
Fig. 1.1 Typical layers of protection for CPI (Adapted from Hendershot, 1999)

Hazard and Operability Study (HAZOP) in addition to traditional methods such as check list, safety review, relative ranking, and "What-if" analysis (Wang, 2004). These methods provide qualitative or quantitative information about the hazards and risks posed by the process, but have not been integrated into process design and optimization framework.

In this section, several inherent safety efforts taken by US corporations and US affiliates of European company are listed:

- Dow Chemical Company – Developed the Dow Fire and Explosion Index (AIChE, 1994a) and the Dow Chemical Exposure Index (AIChE, 1994b) as hazard ranking methodology based on inherent safety principles.

- Exxon Chemical Company – Described inherent safety, health and environment review process based on a life cycle approach (French, Williams, & Wixom, 2004).

- Rohm and Haas Major Incident Prevention Program – used checklist based on inherent safety principles for hazard elimination and risk reduction (Hendershot, 1999).

Safety studies were not only considered by the industries, but also by the US federal government by issuing federal regulations such as Process Safety Management (PSM) of the Occupational Safety and Health Administrations (OSHA), and Risk Management Program (RMP) of the Environmental Protection Agency (EPA).

Overall impression on these efforts is that inherently safer design principles have not been systematically applied. Comparison between traditional efforts and inherently safer design must be performed to understand the importance of inherently safer design principles. As opposed to layer of protection concept, the concept of inherently safer design is to reduce the inherent hazards rather than to control them. There are two things about having lower hazards: they need lesser LOP, less complex LOP and offer lower magnitude of hazards, as shown in Figures 1.3 and 1.4.

Anticipated Potential Incidents   Unanticipated Potential Incidents

LOP for anticipated incidents

Layers do not work for unanticipated mechanisms

Actual Risk

(a)   (b)

Potential Incidents

LOP   Degraded LOP

Actual Risk

(c)
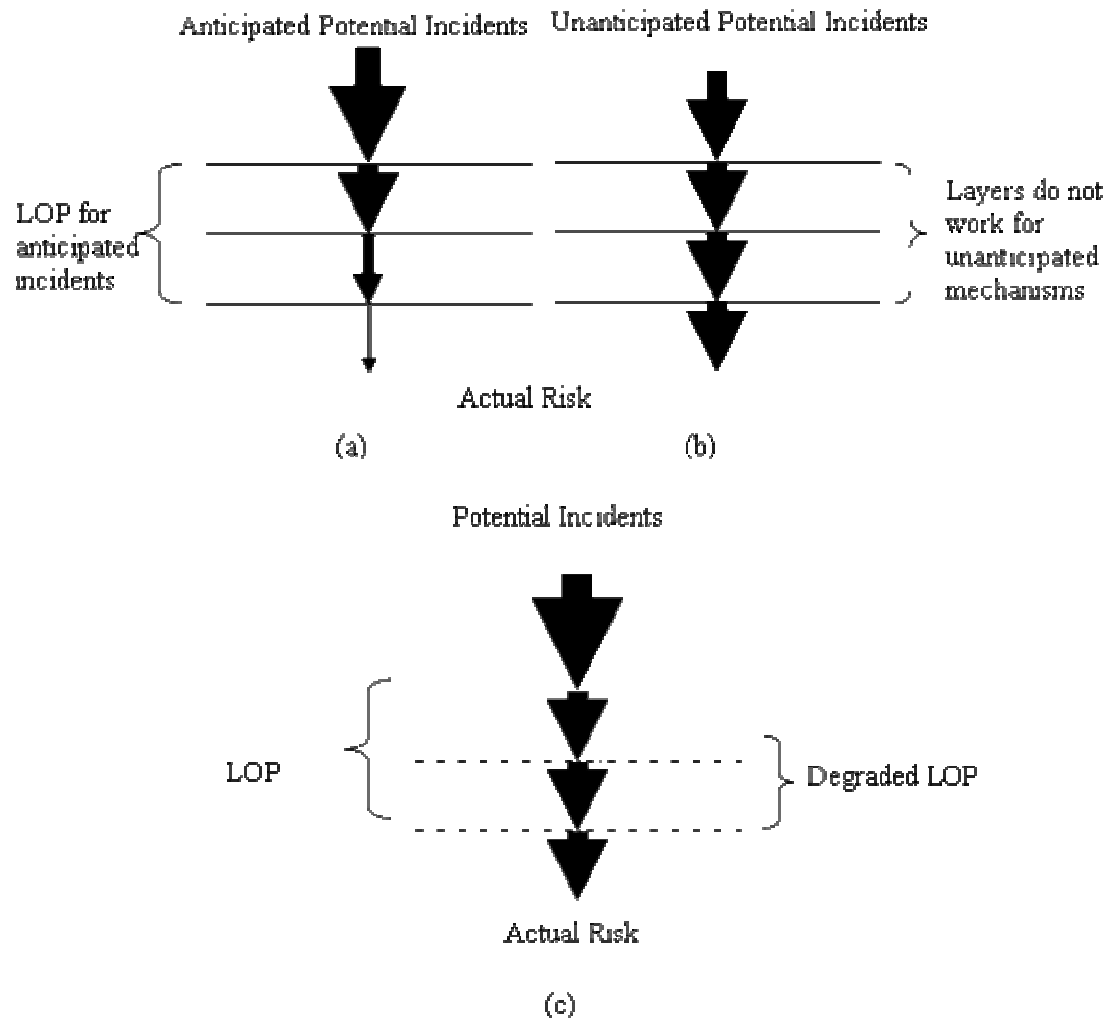
Fig. 1.2. Layers of protection characteristics

(a) LOP reduces the anticipated potential incidents, (b) LOP does not reduce unanticipated potential incidents, (c) degraded LOP does not reduce any potential incidents (adapted from Hendershot, 1999)

Another impression on the traditional approaches is that the efforts focus on hazard identification and control without actively changing the design. This research seeks to integrate inherently safer design concept into process design and optimization using well-accepted hazard identification method, which will be discussed in the next

section. The integration is most effective at the early design stages where there are a lot of degrees of freedom for making changes. In addition, the integration of safety into process design and optimization at the early stages of design will show that safety parameters have active role and give strong feedback to the basic process design strategy.
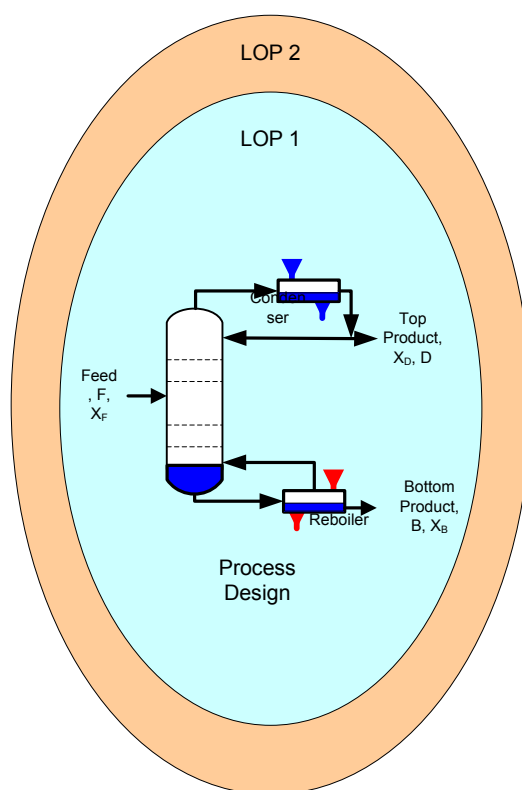
Fig. 1.3 Inherently safer process design requires no or less additional LOP

Potential Incidents

No or Less
LOP needed
by applying
ISD

Actual Risk
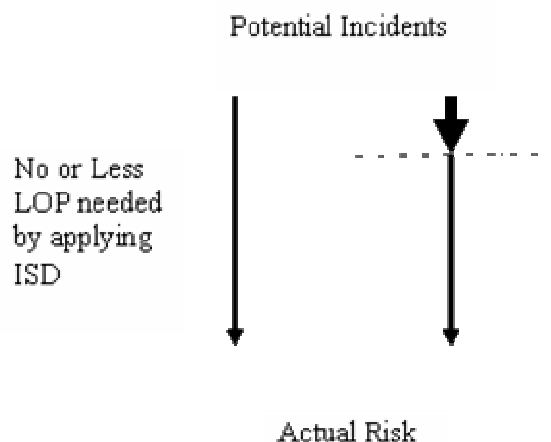
Fig. 1.4 Potential incidents for inherently safer design (adapted from Hendershot, 1999)

1.4 HAZARD INDICES

Most methodologies such as HAZOP, FMEA, and FTA are applicable later in the design stage and require significant funding, special expertise, detailed data and time (Khan, Sadiq, & Amyotte, 2003a). On the other hand, hazard indices offers some characteristics which are applicable to the early stage of design: they can be done quickly, and provide score, penalty, or credit that is easy to interpret, enables comparisons among several design options, and does not require detailed data and special expertise.

There are several hazard indices available as tools for chemical process loss prevention and risk management. Although no index methodology can cover all safety parameters, Dow Fire and Explosion Index (F&EI) and Safety Weighted Hazard Index (SWeHI) are found to be robust (Khan, Sadiq, & Amyotte, 2003a). The F&EI is the most

widely known and used in the chemical industries. The following are indices available in the industries:

- Dow Fire and Explosion Index (F&EI) (AIChE, 1994a) and Dow's Chemical Exposure Hazards (AIChE, 1994b) as tools to determine relative ranking of fire, explosion, and chemical exposure hazards.

- SWeHI as a tool to define fire, explosion, and toxic release hazards (Khan, Sadiq, & Amyotte, 2003a).

- Environmental Risk Management Screening Tools (ERMST®) from Four Elements, Inc. for ranking environmental hazards including air, ground water, surface water pollution (Khan, Sadiq, & Amyotte, 2003a).

- Mond Index as a tool to define fire, explosion, and toxic release hazard (Khan, Sadiq, & Amyotte, 2003a).

- Hazardous Waste Index (HWI) as a tool for flammability, reactivity, toxicity, and corrosivity hazard of waste materials (Khan, Sadiq, & Amyotte, 2003a).

- Transportation Risk Screening Model (ADLTRS®) as a tool for determining risk to people and environment posed by chemical transportation operations (Khan, Sadiq, & Amyotte, 2003a).

- Inherent Safety Index, which was developed by Heikkila (1999) of Helsinki University of Technology. This method classifies safety factors into two categories, chemical and process inherent safety. The chemical inherent safety includes the choice of material used in the whole process by looking at its heat of reaction, flammability, explosiveness, toxicity, corrosivity, and incompatibility

of chemicals. The process inherent safety covers the process equipment and its conditions such as inventory, pressure, temperature, type of process equipment, and structure of the process.

- Overall Inherent Safety Index, which was developed by Edwards & Lawrence (1993) to measure the inherent safety potential for different routes of reaction to obtain the same product.

Fuzzy Logic-based Inherent Safety Index (FLISI), which was developed by Gentile (2004) of Mary Kay O'Connor Process Safety Center at Texas A&M University. One of the major problems in applying inherent safety is that safety mostly based on the qualitative principles that cannot be easily be evaluated and analyzed. The FLISI was an attempt to use hierarchical fuzzy logic to measure inherent safety and provide conceptual framework for inherent safety analysis. The fuzzy logic is very helpful for combining qualitative information (expert judgment) and quantitative data (numerical modeling) by using fuzzy IF-THEN rules.

1.5 PROCESS SAFETY, DESIGN, AND OPTIMIZATION

Currently optimization is performed as an attempt to enhance the process design and the operation conditions of equipment to achieve the largest production, the greatest profit, minimum production cost, the least energy usage, etc. However, neither objective functions nor constraint conditions contain safety parameters in the traditional process optimization. Safety studies are usually performed after process design and optimization.

Safety studies as part of process design and optimization are an iterative procedure and there will not be a single "correct" or "safe" solution. Thus, a "trade off" must be considered, especially when cost benefit analysis is involved. The objective of safety studies is to reduce the frequency and the magnitude of hazardous events as long as economically practicable. All design engineers must be aware of those hazards and make sure that the design is at an acceptable risk level.

Safety is a focal point of any process design that must be balanced with many other factors such as economics, practicality, technology, market, etc (Mansfield & Cassidy, 1994). Safety must be integrated in all aspects of design starting from conceptual to detailed design. Therefore, safety must be integrated into the overall design procedure and presented alongside with other objectives and constraints (Mansfield & Cassidy, 1994).

1.6 OBJECTIVES

It is essential to integrate safety into process design and optimization to achieve inherently safer design. Therefore, this research is to integrate Dow's Fire and Explosion Index into process design and optimization to achieve inherently safer design.

The objectives of this research are:

1. To computerize Dow's Fire and Explosion Index Calculation

2. To generate fire and explosion hazards expressions as a function of operating pressure and the amount of materials in the process units based on the Dow's Fire and Explosion Index.

3. To optimize the reactor and distillation column as case study with economic, performance, and safety parameters as the constraints.

4. To develop a general procedure for integrating safety parameters into process design and optimization.

1.7 CONTENTS OF THIS RESEARCH

To achieve the objectives stated above, there are steps, methods and limitation that are applied to this research. This section discusses the detailed contents of this research.

1.7.1 Design Stage Used in This Research

Table 1.1 provides the procedure of plant design (Mansfield & Cassidy, 1994). This research aims at integrating safety at an early stage of design, specifically process conceptual design.

Table 1.1. The procedures of plant design (Mansfield & Cassidy, 1994)

Decision Point	Key Question/Decisions	Information Used
Initial Specification	What product What throughput	Market research R&D new product ideas
Process Synthesis Route	How to make the product What route, what reactions and materials	R&D chemist's research Known synthesis routes and techniques
Chemical Flowsheet	Flow rate, conversion,	Process synthesis route, lab

Table 1.1. Continued

Decision Point	Key Question/Decisions	Information Used
	pressure, temperature, solvents, etc.	pilot scale trials and knowledge of existing process.
Process Flowsheet	Batch vs continuous operations Unit operation selection Control philosophy	Info above plus process engineering design principles and experience.
Process Conceptual Design	Equipment selection and sizing, inventory of process, overdesign/flexibility, preliminary plant layout, material construction	As above plus equipment suppliers data, raw material data, company design procedures and requirements
Process Detailed Design	Detailed specification based on concept	Process conceptual design and codes/standard and procedures on past project/design

1.7.2 Hazard Analysis Tools and Program Developer

It is essential to integrate process design with a well-accepted hazard index. Dow's Fire and Explosion index (F&EI) 7th edition is employed for fire and explosion hazard analysis. To facilitate the calculation, F&EI calculation is computerized by developing a built in Excel program with Microsoft Visual Basic[®] Application.

After developing a mathematical model of the process under study, optimization is basically solving the model. Hence, an advanced computational solver is needed to run the calculation faster and more efficiently. There are a lot of optimization solvers available. This research employs LINGO[®] optimization software to handle the optimization model because of LINGO [®]'s simplicity, availability, and researcher's familiarity as well.

1.7.3 Integrating Hazard Analysis into Process Design and Optimization

Most safety analyses are qualitative and an equation that relates safety to process parameters is hardly available. On the other hand, optimization requires mathematical model or equations. Hence, it is impossible to design and optimize the process to obtain optimal and inherently safer design without equations. This research generates the equation relating safety to process components from the well-accepted hazard analysis method, Dow's Fire and Explosion Index. Fire and explosion hazard are expressed as a function of pressure and the amount of hazardous chemicals in the process unit. We can also see the effects of having safety as one of the optimization constraints on process design and optimization.

Economic factors are the driving force of the process design and optimization, and are normally used as optimization objective functions. This research will combine process unit performance, economic performance and safety parameter into one optimization case. The resulting design is expected to be optimal, inherently safer, and cost effective.

1.7.4 Case Study: Distillation Column, and Reactor

Basic chemical engineering processes includes mixing, separating, and reaction. Mixing might occur in the reactor and be combined with reaction. A separator is usually used to separate important products produced from a reactor. The reactor-separator system is widely used and should be considered as a whole system since the output of the reactor will define the type and the size of the separator. Therefore, a reactor and distillation column system is used as a case study in this research.

1.8 ORGANIZATION OF THESIS

This thesis consists of seven chapters. Chapter I discusses the motivation, objectives, and contents of this research. Chapter II discusses the hazard analysis method used in this research, Dow's Fire and Explosion Index (FEI). All procedures, limitations, equations, qualitative expressions, options, important guidance, and other detailed data are provided. Chapter III discusses the selection of the reactor and distillation column system, their performance and economic factors in the case study of this research. Chapter IV covers the theory of optimization, kinetic, design, and economic models used

in the optimization of the case study. Chapter V discusses the development of the F&EI program using Microsoft Visual Basic® Application, Microsoft Excel® and LINGO® optimization solver.

Chapter VI recaps the results of this research while Chapter VII gives conclusions and future works that can be done based on this research. The appendix will provide all codes and databases employed in the programming of F&EI calculations.

CHAPTER II

DOW'S FIRE AND EXPLOSION INDEX*

2.1 OVERVIEW

Dow's Fire and Explosion Index (F&EI) is the most widely used hazard index and has been revised six times since 1967. The latest edition (7th edition), which was published in 1994, is employed in this research. AIChE (1994) describes F&EI as the quantitative measurements which are based on historical data, energy potential of the materials under evaluation, and the extent to which loss prevention practices are currently applied. F&EI is valuable as a guide to decide whether it is necessary for process designers to consider other less hazardous materials and/or other process routes (Etowa, Amyotte, Pegg, & Khan, 2002). Moreover, F&EI helps engineers to be aware of the hazards in each process unit while making important decisions in reducing the severity and/or the probability of the potential incident.

F&EI relates process hazards to process information (i.e., process conditions, materials, type of equipment, and other characteristics of the process) in terms of "penalties" and "credit factors". It should be borne in mind that not every penalty is applicable to the process under evaluation so that careful judgment should be made and discussed with the expert if necessary. F&EI is based on the "worst case" which means only the most hazardous material are evaluated at a time in a specific operational state

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*This chapter is a summary of and all tables and Figure 2.1, 2.7, 2.8, 2.9 are reprinted with permission from Dow's Fire & Explosion Index Hazard Classification Giude, by American Institute of Chemical Engineers (AIChE), 1994, AIChE, New York, Copyright 2005 by AIChE. All rights reserved

(i.e., start up, shut down, and normal operation). For example, when a process unit has hazards posed by flammable liquids and dusts, F&EI must be determined based on both flammable liquids and dusts. Then, the higher F&EI and business interruption must be the one that is reported to the management as the worst case.

The details of procedures, guidelines, and equations to determine the penalties and the credit factors of the F&EI are described in the next section. It is very important to understand that all of the information provided in this chapter is primarily a summary of the method given in *Dow's Fire and Explosion Hazard Classification Guide* 7th edition which was published in 1994 by American Institute of Chemical engineers (AIChE).

2.2 DOW'S FIRE AND EXPLOSION INDEX CALCULATIONS

F&EI calculation is composed of steps as shown in Figure 2.1 (AIChE, 1994) and is discussed below. To calculate F&EI, the following documents are required (AIChE, 1994):

1. Plot of the plant/process and/or process flow sheet

2. Replacement cost data for the installed process equipment under study

3. Fire and Explosion Index Hazard Classification Guide, 7th Edition

4. Fire and Explosion Index, Loss Control Credit Factors, Process Unit Analysis Summary, and Manufacturing Unit Risk Analysis Summary Form.

The method starts with the selection the process unit to be evaluated. The user must select the process unit that could pose a significant impact in a potential incident.

Therefore, these important factors must be considered when selecting the process units under evaluation (AIChE, 1994):

- Chemical energy potential (Material factor).

- Quantity of hazardous material.

- Business interruption and capital density (dollars per ft^2).

- Operating pressure and temperature.

- History of fire and explosion incident related to the same type of process unit.

- The importance of the process unit to the whole process.

The F&EI has two components, Process Unit Hazards Factor (F_3) and Material Factor (MF). F_3 consists of General Process Hazards (F_1) and Special Process Hazards (F_2). The F&EI is determined by the Equations (2.1) and (2.2) (AIChE, 1994):

$$F_3 = F_1 \times F_2 \tag{2.1}$$

$$F \& EI = MF \times F_3 \tag{2.2}$$

F_3, F_1, F_2 and MF are discussed hereafter.

2.2.1 Material Factor (MF)

Material factor is the intrinsic rate of potential energy release caused by fire or explosion produced by combustion or chemical reaction. It is the basic starting point of the F&EI calculation and plays a critical role in the magnitude of the F&EI. MF is obtained from reactivity value (N_R) and flammability value (N_F). Appendix A provides a

list of chemicals that are mostly used in the CPI and their MF. For unlisted chemicals,

the data can be obtained from the material safety data sheet (MSDS).
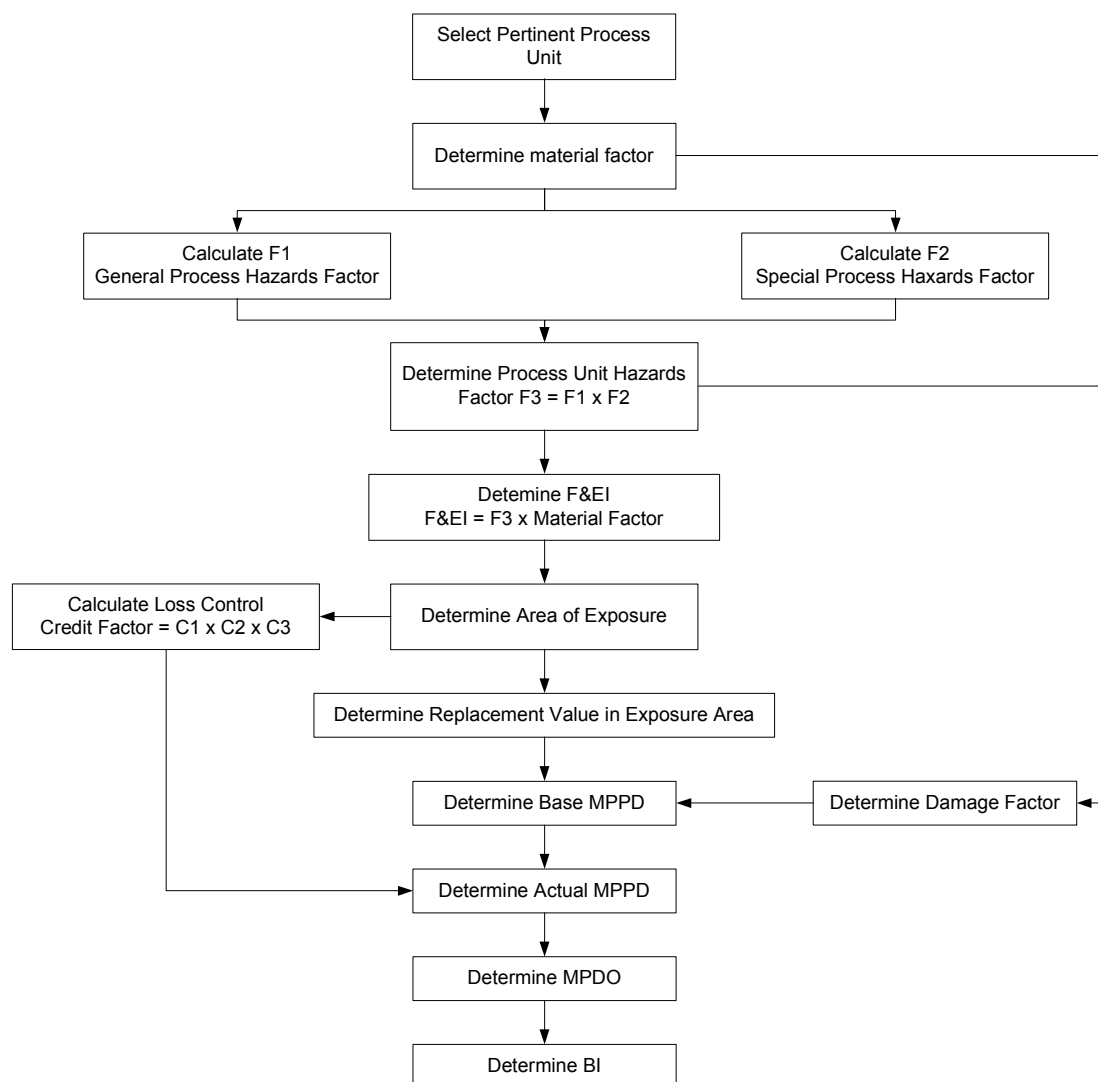
Fig. 2.1 Procedures for calculating F&EI and other risk analysis information (Reproduced with permission. Copyright 1994 AIChE)

Table 2.1 N_F classifications and material factor (MF) determination guide (Reproduced with permission. Copyright 1994 AIChE)

Liquids & Gases Flammablity or Combustibility[1]	NFPA 325 M or 49	Reactivity or Instability				
		$N_R = 0$	$N_R = 1$	$N_R = 2$	$N_R = 3$	$N_R = 4$
Non-combustible[2]	$N_F = 0$	1	14	24	29	40
F.P > 200°F	$N_F = 1$	4	14	24	29	40
100 °F< F.P < 200 °F	$N_F = 2$	10	14	24	29	40
73 °F <F.P > 100°F or F.P < 73 °F and BP ≥ 100 °F	$N_F = 3$	16	16	24	29	40
F.P < 73 °F & BP < 100 °F	$N_F = 4$	21	21	24	29	40
Combustible Dust or Mist[3]				24	29	40
St-1 (Kst ≤ 200 bar m/sec)		16	16	24	29	40
St-2 (Kst = 201-300 bar m/sec)		21	21	24	29	40
St-3 (Kst > 300 bar m/sec)		24	24	24	29	40
Combustible Solids				24	29	40
Dense > 40 mm thick[4]	$N_F = 0$	4	14	24	29	40
Open < 40 mm thick[5]	$N_F = 1$	10	14	24	29	40
Foam, Fiber, Powder, etc[6]	$N_F = 2$	16	16	24	29	40

F.P = Flash Point, Closed cup   B.P = Boiling Point (STP)

Notes:

1: Includes volatile solids

2: Will not burn in air when exposed to T = 1500 °F for five minutes.

3: Kst values are for a 16 liter or larger closed test vessel with strong ignition source

4: Includes wood-2 inches nominal thickness, magnesium ingots

5: includes coarse granular material such as plastic pellets, rack storage, wood pellets,

6: Includes rubber goods (tyre, boots), styrofoam, methocel, etc

If the chemicals are not listed in either MSDS or Appendix A, MF can be determined from N_F and N_R. N_R and N_F are applicable for temperatures up to 140 °F, therefore MF for chemical/material exposed to temperatures higher than 140 °F must be adjusted by "Temperature Adjustment of Material Factor" procedures. The flammability

value (N_F) and the reactivity value (N_R) and their qualitative descriptions are presented

in Table 2.1 and Table 2.2, respectively.

Table 2.2 Qualitative descriptions for determining reactivity value (N_R) (Reproduced with permission. Copyright 1994 AIChE)

$N_R = 0$	Normally stable material even under fire which include: • Material that do not react with water • Material that exhibit exothermic behavior at 572 F < T < 932 F
$N_R = 1$	Normally stable material but unstable at elevated pressure (P) and temperature (T), which include: • Material that change or decompose on exposure to air, light, or moisture • Material that exhibit exothermic behavior at 302 F < T < 572 F
$N_R = 2$	Material that readily go through violent chemical change at elevated P and T, which include • Material that exhibit exothermic behavior at T < 302 ^{o}F • Material that reacts violently or forms potentially explosive material with water
$N_R = 3$	Material that is capable of detonation of explosive decomposition or reaction at the availability of strong intiating source or heated under confinement before initiation. This usually includes: • Material that is sensitive to thermal or mechanical shock at elevated P and T • Material that reacts explosively with water even at unavailability of heat or confinement.
$N_R = 4$	Material that is readily capable of detonation or explosive decomposition or explosive reaction at normal P and T. This includes materials that are sensitive to localized thermal or mechanical shock at normal P and T.

Temperature adjustment is performed only when the temperature of the process unit under study is above 140°F. No adjustment required for material that exhibits reactivity at temperature less than 140°F, has flash point less than 140°F, and is handled at above its flash point at ambient temperature. The temperature adjustment of MF is determined using table 2.3 (AIChE, 1994). "Exotherm start" is the temperature where heat-generating chemical reaction temperature is detected in Accelerating Rate Calorimeter (ARC) or similar calorimeter.

Table 2.3 Material factor temperature adjustment (Reprinted with permission. Copyright 1994 AIChE)

MATERIAL FACTOR TEMPERATURE ADJUSMENT	N_F	St	N_R
A. Enter N_F (St for dusts) and N_R			
b. If Temperature < 140°F, go to "e"			
c. If temperature above flash point or if temperature > 140°F, enter "1" under N_F			
d. If temperature above exotherm start (see paragraph below) or autoignition, enter "1" under N_R			
e. Add each column, but enter 4 when total is 5			
f. Using "e" and tanle 1, determine MF			

2.2.2 Process Unit Hazard Factor (F₃)

Process unit hazard factor incorporates all factors that are likely to contribute to the occurrence of fire and explosion incidents. The numerical value of process unit

hazard factor is determined by general process hazards and special process hazards that are described hereafter.

2.2.2.1 General Process Hazards (F_1)

General process hazard items have historically played an important role in determining the magnitude of potential incidents, and are applicable to most process conditions. General process hazards cover six items, namely, exothermic chemical reactions, endothermic processes, material handling and transfer, enclosed or indoor process units, access and drainage and spill control, although it may not be necessary to apply all of them.

A. Exothermic Chemical Reactions

This item only concerns the reactor where the chemical reactions take place. The chemical reactions are classified into several categories and each receives a different penalty. The chemical reactions considered include:

- Mild exothermic reaction (i.e., hydrogenation, hydrolysis, isomerization, sulfonation, and neutralization) requires a penalty of 0.30.

- Moderate exothermic reaction (i.e., Alkylaton, edterification, addition reactions, oxidation, polymerization, and condensation) requires a penalty of 0.50.

- Critical-to-control exothermic reaction (i.e., halogenation) requires a penalty of 1.00.

- Particularly sensitive exothermic (i.e., nitration) require a penalty of 1.25.

B. Endothermic Processes

All endothermic processes in the reactor require a penalty of 0.2 unless the energy for the endothermic processes is provided by combustion of a solid, liquid or gaseous fuel, whose penalty is 0.4. For example, calcination has a penalty of 0.4, electrolysis has a penalty of 0.20, and pyrolysis or cracking has a penalty of 0.20 if electricity is used as the energy source (and 0.40 if direct fired heat is used).

C. Material Handling and Transfer

This penalty considers the potential fire hazard in process unit during the handling, transfer and warehousing of the material. The loading or unloading process of Class I flammables or LPG type chemicals with the lines that can be connected or disconnected requires a penalty of 0.50. The air present in the centrifuges, batch reactors, or mixers (inerted or not inerted) that might initiate a flammability or reactivity hazards requires a penalty of 0.50. Warehouse storages or yard storages (not storage tanks) involving chemical with potential fire hazards require a penalty of 0.85, 0.65, 0.40, and 0.25 depend on the flammability of the chemicals handled. Utilizing racks without in-rack sprinkler will add 0.20 to the penalty.

D. Enclosed Indoor Process Units

Enclosed area is defined as any roofed area with three or more sides or an area enclosed by a roofless structure with walls on all sides. Open construction is usually

more effective than any mechanical ventilation in an enclosed area unless the ventilation is designed in such a way that all flammables can be collected and dispersed. In such case the penalty will be reduced. The categories are as follows:

- Dust collectors located inside an enclosed area requires a penalty of 0.50.

- Handling flammable fluids at a temperature above their flash point in an enclosed area requires a penalty of 0.30. If more than 1,000 gallons of liquids are handled, the penalty will be 0.45.

- Liquefied petroleum gas (LPG) or any flammable fluids handled at temperatures above their boiling point in an enclosed area require a penalty of 0.60. However, if more than 10,000 lb of liquids are handled, the penalty will be 0.90.

- All of the penalties above will be reduced by 50% if mechanical ventilation is properly designed for the fire hazard.

E. Access

The pertinent process unit must have adequate and ready-to-use access. The minimum requirements look for at least accesses from two sides, at least one access from a roadway and an accessible monitor nozzle during operation. Process areas over 10,000 ft^2 or warehouses over 25,000 ft^2 with inadequate accesses will have 0.35 as the penalty.

F. Drainage and Spill Control

Incidents involving spills of flammable and combustible liquids around or near process equipment have been mostly caused by inadequate design of drainage and spill control. This penalty is given only for material with flash point below 140 ^{o}F or material handled above its flash point. The main factors of the penalty are the total volume of combustible or flammable materials and fire fighting water that are safe enough to handle such amount of materials. The drainage is calculated as the combined volume of the following:

- For process and storage facilities, the total volume used is given by Equation 2.3 (AIChE, 1994):

  Total volume = 100 % largest tank capacity + 10 % next largest tank   (2.3)

- Assume 30 minutes flow rate of fire fighting water or 60 minutes for agricultural chemicals or environmentally harmful chemicals.

The penalty is assigned according to the following guidelines:

- Diking which prevents the spill from reaching other areas but expose all the equipment within the dike or flat areas around process unit will receive a penalty of 0.50.

- If a basin or trench exposes utility lines or does not meet the required distance, the penalty will be 0.50.

- There is no penalty if the diking design requirement below are met:

  - Diking surrounds three sides of an area and direct spills to an impounding basin or unexposed drainage trench.

- Earthen surface requires 2% (min) of the slope to basin or trench while hard surface requires 1%.

- The nearest edge of trench or basin must be separated at least 50ft from the equipment. However, if firewall were installed, the distance can be reduced.

- The impounding basin must have the capacity at least equal to the total volume of the fire fighting water.

2.2.2.2 Special Process Hazards (F_3)

Special process hazards are the factors that play an important role in increasing the probability of a potential incident and comprise of the specific process condition that historically contribute to the major causes of fire and explosion incidents. There are 12 items that are listed as special process hazards and are described below:

A. Toxic Material(s)

Toxic material will cause difficulties and limit the ability of emergency response personnel to reduce the magnitude of the incident.

This penalty depends on health factor (N_H) of the material. For mixture, take the highest N_H. The penalty is given by the Equation (2.4) (AIChE, 1994):

$$Penalty = 0.20 \times N_H \qquad (2.4)$$

N_H is defined in NFPA 704 or NFPA 325 M and attached in Appendix A. Table 2.3 summarizes the N_H according to its qualitative description.

Table 2.4 Qualitative descriptions to determine health factor (N_H) (Reproduced with permission. Copyright 1994 AIChE)

$N_H = 0$	No hazards beyond that normal combustible material offer will occur even on short exposure under fire conditions.
$N_H = 1$	Irritation only on minor residual injury but requires the use of an approved air-purifying respirator when short exposure of the material happens.
$N_H = 2$	Temporary incapacitation, possible residual injury and the use of respiratory protective equipment with independent air supply will occur on intense or short exposure of the material.
$N_H = 3$	Full body protection is required and serious temporary injury will occur when short exposure of the material happens.
$N_H = 4$	Death and major residual injury occur even at very short exposure of the material.

B. Sub-Atmospheric Pressure

This section is applied based on the knowledge that the introduction of air into process equipment (i.e., strippers, compressors, etc) could create or increase the risk of fire or explosion. This will happen only if the inner pressure of the process equipment is lower than the surrounding pressure. This penalty is applied only if the absolute pressure of the process equipment under evaluation is less than 500 mmHg and will receive a penalty of 0.50. If this penalty were applied, do not use the specified penalty given in Section C of "Operation In or Near Flammable Range" and the penalty given in the Section E of "Relief Pressure".

C. Operation in or Near Flammable Range

The introduction of air into process equipment could create fire and/or explosion hazards based on the materials and the equipment conditions. The more hazardous the material and/or process conditions are, the higher the penalty it will receive. However, no penalty is applied if penalty given in section B is applied. This section covers the following conditions:

- Tank storage handling flammable liquid with $N_F = 3$ or 4 and there is a possibility that air can leak into the tank during pump-out or sudden cooling of the tank receives a penalty of 0.50. Open vent or non-inert gas padded operating pressure-vacuum relief receives a penalty of 0.50. Non-inerted storage handling combustible liquids at temperatures above their flash point receive a penalty of 0.50.

- Process equipment that happens to be near flammable range of some material upon instrumental failure receives a penalty of 0.30. Any process that depends on inert purge to have it out of flammable range receives a penalty of 0.30. Barges or tank cars receives a penalty of 0.30.

- Process or operation that will always be at or near flammable range by nature will receive a penalty of 0.80.

D. Dust Explosion

This penalty is applied to any process handling dusts such as transferring, blending, grinding, bagging, and etc. The hazards come from the maximum rate of the

pressure rise and the maximum pressure generated which are both influenced by the particle size. The finer the dust, the higher the maximum rate of the pressure arise and also the higher the maximum pressure generated, hence the higher the hazards. The penalty is based on the particle range size of 90 % of the dust coarser that are measured using Tyler mesh size. Table 2.5 presents penalties for different particle size ranges.

Table 2.5 Dust explosion penalty (Reproduced with permission. Copyright 1994 AIChE)

Particle Size (Micron)	Tyler Mesh Size	Penalty (reduce by 50% in the presence of an inert gas)
175+	60 to 80	0.25
150 to 175	80 to 100	0.50
100 to 150	10 to 150	0.75
75 to 100	150 to 200	1.25
< 75	> 200	2.00

E. Relief Pressure

Operating pressure above atmospheric pressure might cause the release of flammable materials when leakage occurs. Moreover, the rate of release will increase with higher operating pressure. Therefore, this penalty concerns the likelihood of flammable material release upon failures of some components in the process unit. The penalty is determined by the following procedure:

- The penalty for operating pressures in the range of 0 to 1,000 psig is given by Equation (2.5) (AIChE, 1994).

$$Penalty = 0.16109 + \frac{1.61503\,P}{1000} - 1.42879\left(\frac{P}{1000}\right)^2 + 0.5172\left(\frac{P}{1000}\right)^3 \qquad (2.5)$$

With P as the operating pressure.

- The penalty for operating pressure higher than 1,000 psig is given in Table 2.5.

Table 2.6 High pressure penalty for flammable & combustible liquids (Reproduced with permission. Copyright 1994 AIChE)

Pressure (psig)	Pressure (kPa gauge)	Penalty
1,000	6,895	0.86
1,500	10,343	0.92
2,000	13,790	0.96
2,500	17,238	0.98
3,000 to 10,000	20,685 to 69,950	1.00
> 10,000	> 68,950	1.50

F. Low Temperature

This section is based on the fact that carbon steel or other metal might be brittle when exposed to a temperature at or below their ductile/brittle transition temperatures. No penalty needs to be applied if there is no possibility of such temperatures. If the process utilizes carbon steel construction and operates at or below its ductile/brittle transition temperature, the penalty is 0.30. Other materials receive a penalty of 0.20.

G. Quantity of Flammable/Unstable Material

This section concerns the effects of the quantities of flammable and unstable materials on the hazard. There are three categories, calculated separately by considering only one applicable category based on the material selected as the MF, and discussed hereafter.

• Liquids or Gases in Process

This section considers the quantity of a material that may be spilled and creates a fire, explosion, or a reactive chemical event. The penalty is based on the flow rate of the material for 10 minutes, where the larger value between the quantity of material in the process unit and the quantity of material in the largest connected unit is applied. The penalty is determined by using Figure 2.2 or given by Equation (2.6) (AIChE, 1994):

$$Log(Y) = 0.17179 + 0.42988(LogX) - 0.37244(LogX)^2 \qquad (2.6)$$

$$+ 0.17712(LogX)^3 - 0.029984(LogX)^4$$

where Y is the penalty and X is total energy in the process (BTU x 10^9). This penalty applies only to these materials:

- • Flammable and combustible liquids with flash point < 140°F.

- • Flammable gases and liquefied flammable gases.

- • Combustible liquids with F.P > 140 °F

- • Reactive chemicals.
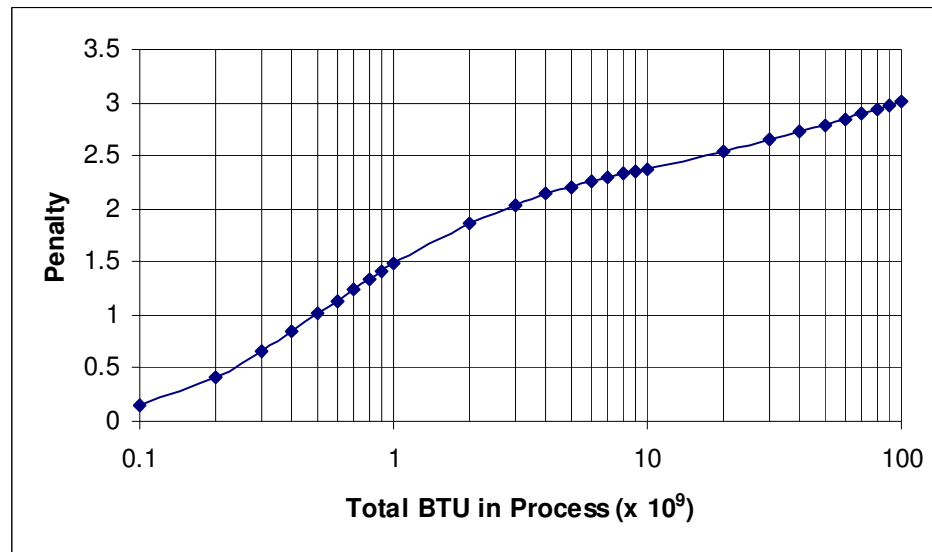
Fig. 2.2. Penalty for liquids or gases in process (Plot of Equation 2.6)

• **Liquids or Gases in Storage (Outside the Process Area)**

This penalty considers flammable and combustible fluids in storage (i.e., drums, tanks, material in tank farms, portable container, containers, etc) where no process is involved. There are three categories which depend on the amount of the material, the type of the liquid/gases and the heat of combustion (H_C). The penalty is determined by using Figure 2.3 or given by Equation (2.7), (2.8) and (2.9) (AIChE, 1994):
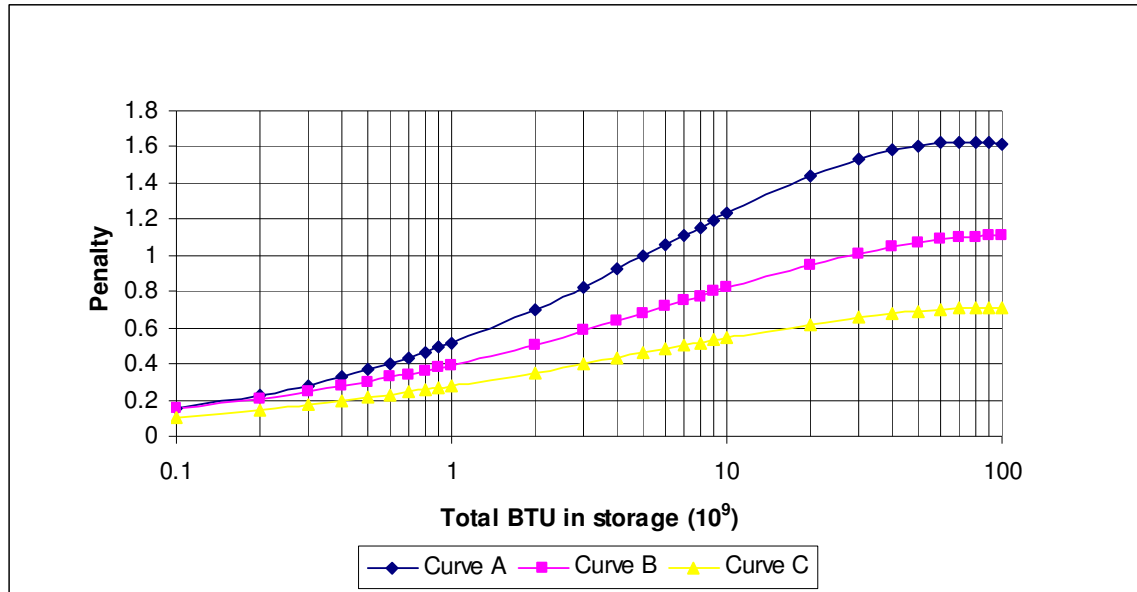
Fig. 2.3. Quantity of flammable/unstable material penalty to liquids or gases in storage (Plot of Equations (2.7), (2.8), and (2.9))

Curve A: Liquefied Gases

$$Log(Y) = -0.289069 + 0.472171(LogX) - 0.074585(LogX)^2 + 0.018641(LogX)^3 \quad (2.7)$$

Curve B: Class I Flammable Liquids (F.P < 100 ^{o}F)

$$Log(Y) = -0.403115 + 0.378703(LogX) - 0.046402(LogX)^2 - 0.015379(LogX)^3 \quad (2.8)$$

Curve C: Class Combustible Liquids (100 ^{o}F < F.P < 140 ^{o}F)

$$Log(Y) = -0.558394 + 0.363321(LogX) - 0.057296(LogX)^2 + 0.057296(LogX)^3 \quad (2.9)$$

where Y is the penalty and X is total energy in the process (BTU x 10^9).

• **Combustible Solids in Storage/Dust in Process**

This penalty covers the quantities of stored solids and dusts when they are involved as the basis for the MF. The penalty based on the density of the material, the ease of ignition, and the ability to sustain a flame. The penalty is determined by the Figure 2.4 or Equations (2.10) and (2.11) (AIChE, 1994):
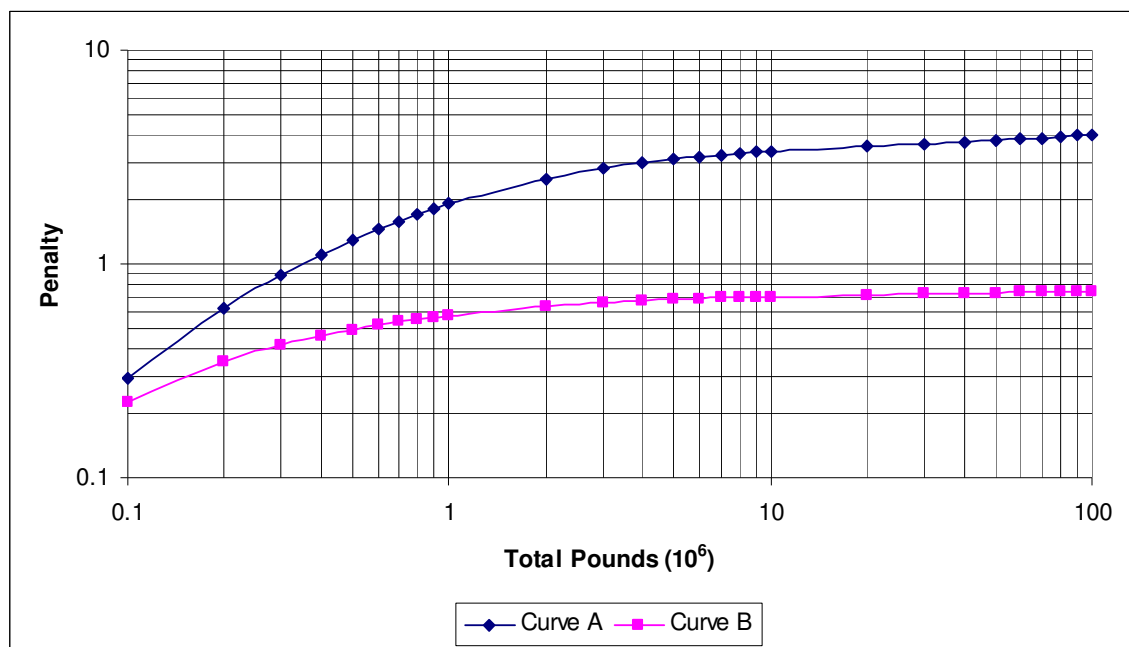
Fig. 2.4. Quantity of flammable/unstable material penalty to combustible solids in storage/dust in process (Plot of Equations (2.10) and (2.11))

Curve A: Material with Density < 10 lb/cu ft

$$LogY = 0.280423 + 0.464559 \times LogX \qquad (2.10)$$

$$-0.28291 \times (LogX)^2 + 0.066218 \times (LogX)^3$$

Curve B: Material with Density > 10 lb/cu ft

$$LogY = -0.358311 + 0.459926 \times LogX \tag{2.11}$$

$$-0.141022 \times (LogX)^2 + 0.02276 \times (LogX)^3$$

where Y is the penalty and X is total amount in the process (BTU x 10^6).

H. Corrosion and Erosion

The corrosion rate is the sum of the external and internal corrosion rate. These following penalties should be applied:

- If the corrosion rate<0.005 in/yr with risk of pitting or local erosion, the penalty is 0.10

- If 0.127 mm/yr < Corrosion rate < 0.254 mm/yr, the penalty is 0.20.

- If the corrosion rate > 0.254 mm/yr, the penalty is 0.50.

- If the risk of stress-corrosion cracking might develop, the penalty is 0.75. This occurs in process areas contaminated by chlorine vapor over prolonged periods.

- If lining is required to avoid corrosion, the penalty is 0.20. However, this is not the case if the lining is simply to protect the product from developing color.

I. Leakage-Joints and Packing

The leaking of flammable or combustible fluids can be found in gaskets, seals of joints, shafts or packings, especially where thermal and pressure cycling occurs. The

penalty is given according to the design of the process unit. These penalties should be applied:

- If it is possible to develop a minor leakage at the pump and gland, the penalty is 0.10.

- If the leakage occurs regularly at pumps, compressors, and flange joints, the penalty is 0.30.

- Processes that have the potential to undergo thermal and pressure cycling receive a penalty of 0.30.

- If the material is penetrating in nature or abrasive slurry that causes problems with sealing and if the process unit uses rotating shaft seal or packing, the penalty is 0.40.

- Any process unit with sight glasses, bellows assemblies, or expansion joints receive a penalty of 1.50

J. Use of Fired Equipment

This penalty considers the additional hazards offered by fired equipment. It is decided based on distances from probable leak points to air intake of the fired equipment and is determined by using Figure 2.5 or given by Equation (2.12) and (2.13) (AIChE, 1994):

- Curve A-1 is used for material released above its flash point and for combustible dust.

$$LogY = -3.3243\left(\frac{X}{210}\right) + 3.75127\left(\frac{X}{210}\right)^2 - 1.42523\left(\frac{X}{210}\right)^3 \tag{2.12}$$

- Curve A-2 is for material released above its boiling point

$$LogY = -0.3745\left(\frac{X}{210}\right) - 2.70212\left(\frac{X}{210}\right)^2 + 2.09171\left(\frac{X}{210}\right)^3 \tag{2.13}$$

where Y is the penalty and X is distance (ft).
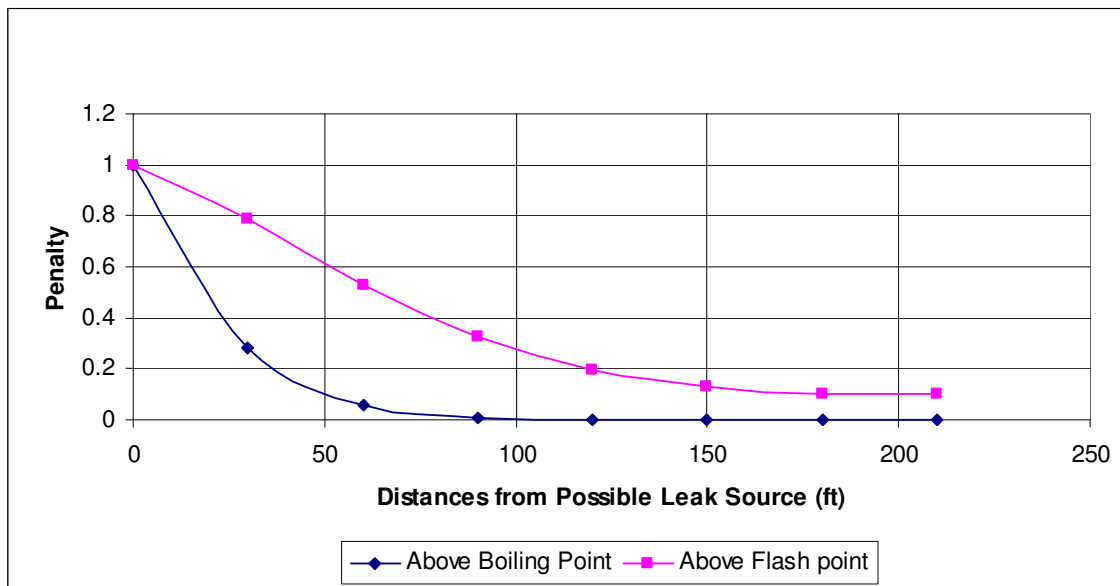
Fig. 2.5. Quantity of flammable/unstable material penalty to fired equipment (Plot of Equations (2.12) and (2.13))

If the fired equipment itself is being evaluated, then the distance will be zero. If the equipment is heating a flammable or combustible material, the penalty will be 1.00.

K. Hot Oil Heat Exchange System

This penalty is determined based on the quantity and the temperature of the heat exchange fluids used in the unit. Penalty is not applied to the non-combustible hot oil or to combustible fluids used below their flash point. The quantity of the fluids used in calculating the penalty is the smaller value between 15 minutes of spill or the hot oil inventory in an active circulating hot oil system. Table 2.7 summarizes the penalty for different quantity of hot oils in heat exchange systems.

Table 2.7 Hot oil heat exchange system penalty (Reproduced with permission. Copyright AIChE 1994)

Quantity, Gallons	Above Flash Point Penalty	At or Above Boiling Point Penalty
< 5,000	0.15	0.25
5,000 to 10,000	0.30	0.45
10,000 to 25,000	0.50	0.75
> 25,000	0.75	1.15

L. Rotating Equipment

This penalty concerns about the hazard offered by large rotating equipment such as pumps, compressors, agitators, circulating pumps, and centrifuges. The penalty is defined based on the statistical evidence available for some rotating equipment at a certain size that is likely to contribute to a potential incident.

Process units having compressors in excess of 600 hp and/or pumps in excess of 75 hp receive a penalty of 0.50. The same penalty is given to agitator (mixers) and circulating pumps in which failure creates exothermic reactions when lack of cooling occurs and also to other large high speed rotating equipment with substantial loss history.

2.2.3 The Determination of Fire and Explosion Index

The Dow Fire and Explosion Index (F&EI) is the product of the Process Unit Hazard Factor (F1) and the Material Factor (MF). Then, the degree of hazards (severity) of the process evaluated can be determined by using Table 2.8.

Table 2.8 Degree of Hazard for F&EI (Reproduced with permission. Copyright AIChE 1994)

F&EI Index Range	Degree of Hazards
1 – 60	Light
61 – 96	Moderate
97 – 127	Intermediate
128 – 158	Heavy
159 – up	Severe

2.2.4 Loss Control Credit Factors

These factors represent the loss control (protective) features that have been historically and statistically proven beneficial in preventing or limiting serious incidents. The basic thinking of using this credit factor is different from the F&EI value. High

F&EI shows that process under evaluation contains high hazards while high loss control credit factor shows that there is less chance for the incident to occur. Therefore, a good design is usually defined as one which has the lowest possible of the F&EI and the highest possible loss control credit factor.

There are three categories of loss control credit factors: Process Control (C_1), Material Isolation (C_2) and Fire Protection (C_3). If no credit factor is applied to a particular item, the credit factor is 1.0 for that item. The total credit factor is given by Equation (2.14) (AIChE, 1994):

$$C_{total} = C_1 \times C_2 \times C_3 \qquad\qquad (2.14)$$

The next sections list items in all categories.

2.2.4.1 Process Control Credit Factors (C_1)

Process control credit factors consist of:

- Emergency Power – credit factor of 0.98

    This credit factor is applicable only if emergency power is available to control an incident.

- Cooling

    If process cooling system is able to handle 10 minutes of normal cooling during abnormal situation, the credit factor is 0.99. If a backup cooling system is available to handle 150% of cooling requirement for at least 10 minutes, the credit factor is 0.97.

- Explosion Control

    If explosion suppression systems are employed on dust or vapor-handling equipment, the credit factor is 0.84. If the overpressure relief systems utilize rupture disks or explosion-relieving vents that protect the process unit from abnormal conditions, the credit factor is 0.98.

- Emergency Shutdown – credit factor of 0.96 to 0.99

    If redundant system is able to activate and initiate shutdown sequence in the event of an incident, the penalty is 0.98. If rotating equipment (i.e., compressors, turbines, fans) is designed with vibration detection, the credit factor is 0.99.

- Computer Control – credit factor of 0.93 to 0.99

- Inert Gas – credit factor of 0.94 to 0.96

- Operating Instruction/Procedures – 0.91 to 0.99

- Reactive Chemical Review – 0.91 to 0.98

- Other Process Hazards Analysis – 0.91 to 0.98

2.2.4.2 Material Isolation Credit Factor (C_2)

- Remote Control Valves – credit factor of 0.96 to 0.98

- Dump/Blowdown – credit factor of 0.96 to 0.98

- Drainage – credit factor of 0.91 to 0.97

- Interlock – credit factor of 0.98

2.2.4.3 Fire Protection Credit factor (C_3)

- Leak Detection – credit factor of 0.94 to 0.98

- Structural Steel - credit factor of 0.95 to 0.98

- Fire Water Supply - credit factor of 0.94 to 0.97

- Special Systems – credit factor of 0.91

- Sprinkler Systems – credit factor of 0.74 to 0.97

  Credit factors for wet and dry pipes used in indoor manufacturing areas and

  warehouses are shown in Table 2.9

Table 2.9 Credit Factors for wet pipe and dry pipe used in indoor manufacturing areas and warehouses (Reproduced with permission. Copyright AIChE 1994)

	Design		Credit Factor	
Occupancy	**Gpm/ft^2**	**Lpm/m^2**	**Wet Pipe**	**Dry Pipe**
Light	0.15 – 0.20	6.11 – 8.15	0.87	0.87
Ordinary	0.21 – 0.34	8.56 to 13.8	0.81	0.84
Extra Hazard	≥ 0.35	≥ 14.3	0.74	0.81

- Water Curtain - credit factor of 0.97 to 0.98

- Foam - credit factor of 0.92 to 0.97

- Hand Extinguisher/Monitors – credit factor of 0.03 to 0.98

- Cable Protection – credit factor of 0.94 to 0.98

2.2.5 Process Unit Risk Analysis Summary

To identify equipment that potentially contributes to the occurrence of an incident and to communicate it to the top management in the company, engineers can use "process unit risk analysis summary", which presents hazards based on F&EI and business interruption of particular equipment. This section discusses how to determine the business interruption.

2.2.5.1 The Fire and Explosion Index (F&EI)

All calculation is based on F&EI calculation presented in Section 2.2. The higher the F&EI value, the higher the hazard thus the higher the business interruption.

2.2.5.2 The Radius of Exposure

This radius of exposure is the radius in which all equipment in the radius range will be exposed to the potential incident. For large pieces of equipment, the radius starts from the surface of the equipment while for small equipment the radius starts at the center of the item considered. The F&EI is converted into the radius of exposure by using Equation (2.15) (AIChE, 1994):

$$Radius\ of\ Exposure\ (ft) = 0.84 * (F\ \&\ EI) \qquad (2.15)$$

2.2.5.3 The Area of Exposure

The area of exposure is determined from the radius of exposure using the area of a circle formulation, as shown in Equation (2.16) (AIChE, 1994).

$$Area\ of\ Exposure\ \left(ft^2\right) = \pi\ R^2 \qquad\qquad (2.16)$$

Theoretically, any equipment inside the area of exposure range will be exposed to the hazard. Better assumption can also be done by taking cylindrical volume over the equipment under evaluation with the height equal to the radius of exposure.

2.2.5.4 Value of the Area of Exposure

The value of the area of exposure is calculated from the replacement values of all the property contained within it and the inventory of the material, as shown in Equation (2.17) (AIChE, 1994).

$$replacement\ value = original\ \cos t \times 0.82 \times escalation\ factor \qquad (2.17)$$

The factor 0.82 is the allowance for items that is not subjected to loss or replacement (i.e., site preparation, roads, foundation). This factor is flexible to change when more accurate factor is available. The escalation factor is the chemical engineering plant cost index (CEPCI) which is different for each year and is available in several chemical engineering journals.

2.2.5.5 Damage Factor

Damage Factor corresponds to the overall effects resulting from a release of energy contained in process unit and is calculated from the process unit hazards factors (F_3) and the material factors (MF). For MF equal to 1, 4, 10, 14, 16, 21, 24, 29, and 40 and F_3 less or equal to 8, the damage factors are calculated by the Equations (2.18) – (2.26) (AICHE, 1994). For F_3 greater than 8, use F_3 equal to 8.

Material Factor of 1:

$$Y = 0.003907 + 0.002957 * X + 0.004031 * X^2 - 0.00029 * X^3 \qquad (2.18)$$

Material Factor of 4:

$$Y = 0.025817 + 0.019071 * X - 0.00081 * X^2 - 0.00029 * X^3 \qquad (2.19)$$

Material Factor of 10:

$$Y = 0.098582 + 0.017596 * X + 0.000809 * X^2 - 0.000013 * X^3 \qquad (2.20)$$

Material Factor of 14:

$$Y = 0.20592 + 0.017596 * X + 0.007628 * X^2 - 0.00057 * X^3 \qquad (2.21)$$

Material Factor of 16:

$$Y = 0.256741 + 0.019886 * X + 0.011055 * X^2 - 0.00088 * X^3 \qquad (2.22)$$

Material Factor of 21:

$$Y = 0.340314 + 0.076531 * X + 0.003912 * X^2 - 0.00073 * X^3 \qquad (2.23)$$

Material Factor of 24:

$$Y = 0.395755 + 0.096443 * X - 0.00135 * X^2 - 0.00038 * X^3 \qquad (2.24)$$

Material Factor of 29:

$$Y = 0.484766 + 0.094288 * X - 0.00216 * X^2 - 0.00031 * X^3 \qquad (2.25)$$

Material Factor of 40:

$$Y = 0.554175 + 0.080772 * X + 0.000332 * X^2 - 0.00044 * X^3 \qquad (2.26)$$

2.2.5.6 Base Maximum Probable Property Damage (Base MPPD)

Base MPPD is the value (in US dollar) of the plant equipment evaluated or property losses within the theoretical area of exposure. It is based on the value of the area of exposure and the damage factor, as shown in Equation (2.27) (AIChE, 1994).

$$Base\ MPPD = Damage\ Factor \times Value\ of\ area\ of\ \exp osure \qquad (2.27)$$

2.2.5.7 Loss Control Credit Factor

This is calculated based on the section 2.2.4.

2.2.5.8 Actual Maximum Probable Property Damage (Actual MPPD)

Having loss control (protective) features in the equipment will reduce the magnitude of the incident, thus the damages. Therefore, base MPPD must be modified according to the loss control features to estimate actual MPPD, which are more reasonable property damage losses. The actual MPPD is determined by Equation (2.28) (AIChE, 1994).

$$Actual\ MPPD = Loss\ Control \times Base\ MPPD \qquad (2.28)$$

2.2.5.9 Maximum Probable Days Outage (MPDO)

The business interruption consists not only of property damages but also of product and inventory losses that will determine the value of MPDO. For example, losses depend on the ability to make up the lost product at distant facilities, the ability to

get one-of-a-kind equipment, and loss of profits due to the shutdown of the plant. More days of outage result in more MPDO, thus more business interruptions.

If such real data for equipment and days of outage are not available, MPDO is calculated by using Figure 2.6 or by using Equations (2.29), (2.30) and (2.31) (AIChE, 1994). For the equipment which is hard to get, the upper 70 % probability limit is used. For in-stock equipment, the lower 70 % probability limit is applied.

Upper 70 % Probability Limit

$$LOG(Y) = 1.550233 + 0.598416 * LOG(X) \qquad (2.29)$$

Normal

$$LOG(Y) = 1.325132 + 0.592471 * LOG(X) \qquad (2.30)$$

Lower 70 % probability Limit

$$LOG(Y) = 1.045515 + 0.610426 * LOG(X) \qquad (2.31)$$

2.2.5.10 Business Interruption (BI)

Business interruption in the event of incident is calculated by Equation (2.32) (AIChE, 1994):

$$BI\ (US\ \$) = \frac{MPDO}{30} \times VPM \times 0.7 \qquad (2.32)$$

VPM is the value of the months and 0.70 represents the fixed cost plus profit.
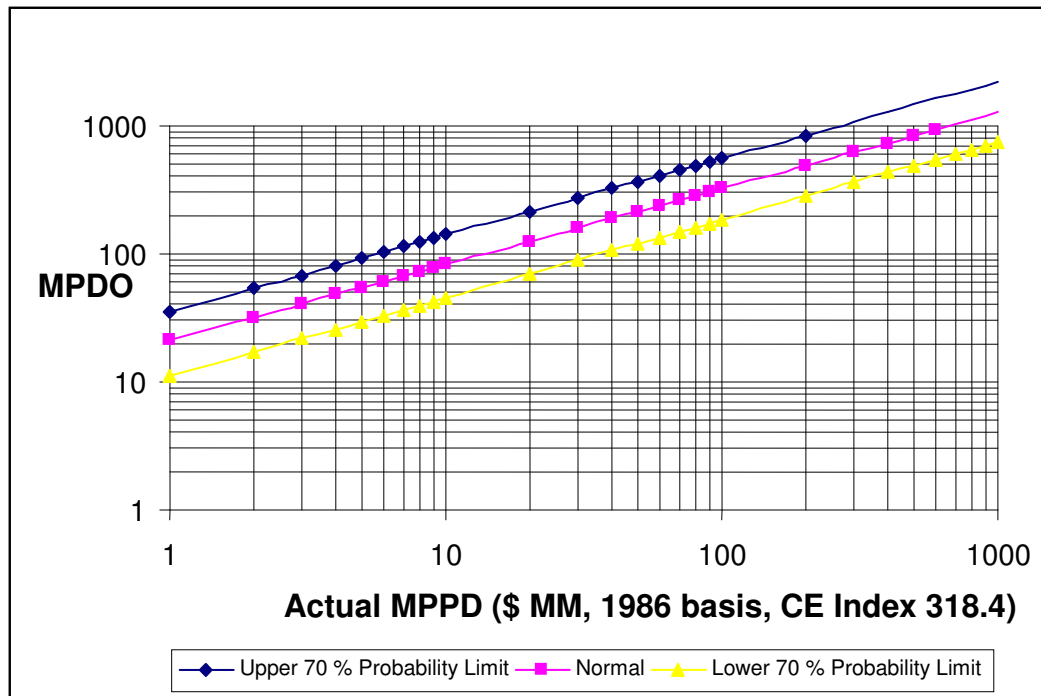
Fig. 2.6. Determining MPDO from Actual MPPD (Plot of Equations (2.29), (2.30), and (2.31))

2.3 FIRE AND EXPLOSION INDEX FORM

All values from F&EI calculation are submitted to the Fire and Explosion Index form, Loss Control Credit factors form, and Process Unit Analysis Summary form. This is intended to be a summary of the calculations. The forms are shown in Figures 2.7, 2.8, and 2.9.

Dow's Fire and Explosion Index is the hazards analysis method used in this research. It is very important to have design equations for each of the equipment under evaluation available in order to integrate the safety parameters into process design and optimization. The next chapter, Chapter III, provides the design equations used in this research.

PROCESS UNIT ANALYSIS SUMMARY

1	Fire and Explosion Index (F&EI)		
2	Radius of Exposure		ft or m
3	Area of Exposure		ft^2 or m^2
4	Value of area of exposure	$MM	
5	Damage Factor		
6	Base Maximum Probable Property Damage (Base MPPD) [4 x 5]	$MM	
7	Loss Control Credit Factor		
8	Actual Maximum Probable Property Damage (Actual MPPD) [6 x 7]	$MM	
9	Maximum Probable Days Outage (MPDO)		
10	Business Interruption (BI)	$MM	

Fig. 2.7. Process unit analysis summary form (Reproduced with permission. Copyright AIChE 1994)

1. Process Control Credit Factors (C1)

	Feature	Credit Factor Range	Credit Factor Used
A	Emergency Power		0.98
B	Cooling		0.97
C	Explosion Control		0.84
D	Emergency Shutdown		0.99
E	Computer Control		0.97
F	Inert Gas		0.94
G	Operating Instructions/Procedures		0.97
H	Reactive Chemical Review		1
I	Other Process Hazard Analysis		0.94
		C_1 Value	**0.66**

2. Material Isolation Credit Factor (C_2)

	Feature	Credit Factor Range	Credit Factor Used
A	Remote Control Valve		1
B	Dump/Blowdown		1
C	Drainage		0.97
D	Interlock		0.98
		C_2 Value	**0.95**

3. Fire Protection Credit Factor (C_3)

	Feature	Credit Factor Range	Credit Factor Used
A	Leak Detection		0.94
B	Structural Steel		0.98
C	Fire Water Supply		0.97
D	Special Systems		1.00
E	Sprinkler Systems		0.92
F	Water Curtains		0.97
G	Foam		0.94
H	Hand Extinguishers/Monitors		0.98
I	Cable Protection		0.94
		C_3 Value	**0.69**

Loss Control Credit Factor = C_1 x C_2 x C_3 = | **0.43**

Fig. 2.8. Loss Control credit factor form (Reproduced with permission. Copyright AIChE 1994)

Material Factor

		Penalty Factor Range	Penalty Factor Used
1	**General Process Hazards**		
	Base Factor		
	A. Exothermic Chemical reactions		
	B. Endothermic Processes		
	C. Material Handling and Transfer		
	D. Enclosed or Indoor Process Units		
	E. Access		
	F. Drainage and Spill Control		
2	**Special Process Hazards**		
	Base Factor		
	A. Toxic Material(s)		
	B. Sub-Atmospheric Pressure (, 500 mmHg)		
	C. Operation In or Near Flammable Rang __*__ Inerted _____ Not Inerted		
	1. Tank Farms Storage Flammable Liquids		
	2. Process Upset or Purge Failure		
	3. Always in Flammable Range		
	D. Dust Explosion		
	E. Pressure Operating Pressure _____788.5_ psig or kPa gauge		
	Relief Setting _____850_____ psig or kPa gauge		
	F. Low Temperature		
	G. Quantity of Flamable/Unstable Material: Quantity _____ lb/kg		
	Hc = _____ BTU/lb or kcal/kg		
	1. Liquids or Gases in Process		
	2. Liquids or Gases in Storage		
	3. Combustible Solids in Storage, Dust in Process		
	H. Corrosion and Erosion		
	I. Leakage-Joints and Packing		
	J. Use of Fired Equipment		
	K. Hot Oil Heat Exchange System		
	L. Rotating Equipment		
	Special Process Hazards Factor (F2)		
	Process Unit Hazards Factor (F1 x F2) = F3		
	Fire and Explosion Index (F3 x MF = F&EI)		

Fig. 2.9. Fire and Explosion Index Form (Reproduced with permission. Copyright AIChE 1994)

CHAPTER III

REACTOR -DISTILLATION COLUMN DESIGN

AND ECONOMIC PARAMETER

3.1 BACKGROUND

3.1.1 Reactor

Basic chemical engineering processes include reaction, separation, and mixing. Reactors are used in the industry to conduct commercial scale reactions. There are several characteristics of reactor and its reaction. Reactor physical dimension depends on the required structure to withstand the operating conditions (pressure, temperature, flow rate, etc) and the rate of the reaction. The size of a reactor is large not because the desired output is large but due to the low reaction rate and/or the low conversion (Kletz, 1991). Low conversion means that more un-reacted reactant must be recycled; also, larger inventory is needed. It is common in the chemical industries that reactor is followed by separator to separate the un-reacted raw materials and the specified products. Thus, reactor-distillation column system is a common system used in the chemical industries. Reactions are slow because of poor mixing or inherently slow reaction. From an inherently safer design (ISD) point of view, vapor phase reaction is preferable than liquid phase because the vapor density is less than that of liquid (Kletz, 1991). Therefore, the rate of leak through a hole of a certain size is lower.

In performing economic analysis of a reactor, the separator should be included since there is trade-off between reactor-separator systems as shown in Figure 3.1.

Economic balance between a high reactor cost at high conversion and a high separation cost at low conversion will determine the optimum reactor conversion. Therefore, it is necessary to have a procedure to improve reactor performance and/or reactor-distillation column system to produce desired products while in the range of acceptable economic profit and safety level. The design equations and economic parameters of a reactor are presented in this chapter.
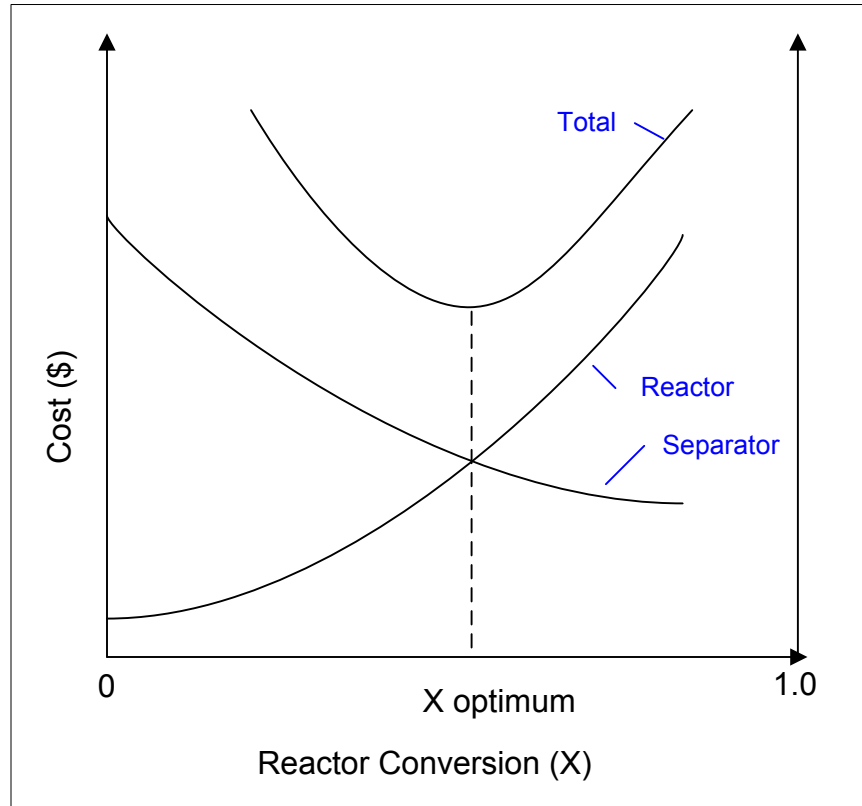
Fig.3.1. Costs of reactor and distillation column as a function of reactor conversion (Smith, 1995)

3.1.2 Distillation Column

Distillation column is probably the most widely for separation process in the chemical industries. Its application ranges from alcohol purification to crude oil fractionation. Distillation column separates materials based on the volatility of the components. The component with greater volatility will be easier to separate. A simple distillation column is shown in Figure 3.2. The rectifying section is the section above the feed where the concentration of the more volatile components is increased to produce the top products. The stripping section is located below the feed where the more volatile components are stripped by the liquid then the bottom products produce. The vapor will flow upward counter-currently while the liquid will flow downward. Liquid and vapor are contacted on plates or packing inside the column.

Equations to model distillation column must be developed before optimizing distillation column. These equations are described in section 3.3.

3.1.3 Economics as Objective Functions of Optimization

Economics as objective functions of optimization consists of two major components: operating cost and capital cost (Edgar, Himmelblau, & Lasdon, 2001). Capital cost estimation is available at the following four stages of increasing levels of accuracy (Seider, Seader, & Lewin, 2004):

- Order-of-magnitude estimate – based on laboratory data to estimate the types of equipment and how to organize the equipment in order to produce chosen products. Only two things are needed, production rate in lb/year and flow sheet

considering gas compressors, reactors, and separation equipment only. Heat exchanger and liquid pump are not included in the estimation. Mass balance and equipment sizing are not required either. The accuracy of this method is ± 50 %.

- Study estimate – based on preliminary plant design. This estimation uses method of Lang (Seider, Seader, & Lewin, 2004). The accuracy of this method reaches ±35 %. The detailed description about the Lang method is described later in this chapter.

- Preliminary estimate – based on detailed design (P&ID) and performed after optimal design has been achieved. More time is required to perform this method but the accuracy is increased to ± 20 %.

- Definite estimate – based on detailed process design, detailed drawings, cost estimates, and other data to have accurate cost accounting. It is intended for construction.

Total production costs consist of direct production cost (operating cost), fixed charges, plant overhead costs, administrative expenses, and distribution and marketing expenses (Peters & Timmerhaus, 1991). The optimization variables in this research that are related to total production cost are operating cost, with the capability to include other cost if data are available. Operating cost depends on several factors such as raw materials, operating man, operating supervision, royalties, utilities, etc. However, this research only uses the raw materials and utilities cost as the operating cost to demonstrate the proposed methodology.

3.2 THE METHOD OF LANG

The method of Lang estimates capital cost using overall factors that multiply the cost of f.o.b purchase cost of the equipment. The f.o.b purchase cost is the cost of the equipment paid by the buyer where the seller has the obligation to deliver the equipment to a certain place for transfer, not directly to the plant site. The data needed for this method are process design with its material and energy balances, equipment sizing, and the material of construction. The accuracy of the method of Lang is ± 35 %.

The method of Lang proceeds by steps as follows (Seider, Seader, & Lewin, 2004):

- Prepare an equipment list and their size, the materials of construction, the design temperature, and the design pressure.

Calculate the total permanent investment (C_{TCI}) by using Equation (3.1) (Seider, Seader, & Lewin, 2004):

$$C_{TCI} = 1.05 f_{L_{TCI}} \Sigma \left(\frac{I_i}{I_{bi}} \right) C_{P_i} \tag{3.1}$$

with C_{TCI} represents total permanent investment, $f_{L_{TCI}}$ as Lang's factors, $\dfrac{I_i}{I_{bi}}$ is the ratio of cost index, and C_{P_i} is the total f.o.b purchase cost of the equipment. Lang factor recommended by Peters & Timmerhaus (1991) for fluids processing chemical plants is 5.7, for solids-fluids processing plants is 4.9, and for solids processing plants is 4.6. These numbers are based on a value of 100 for the total delivered cost, which is 1.05 times the f.o.b purchase cost.

In this research, f.o.b purchase cost for distillation column and reactor are estimated before using method of Lang and determining the total investment cost, as shown in the following section. In addition, the technical design equations are also described.

3.3 DISTILLATION COLUMN AND REACTOR DESIGN EQUATIONS

3.3.1 Column Distillation Design Equations

The design of distillation column consists of many procedures and equations and commercial simulators have been developed. However, it is very important to understand the basic design calculations of distillation column, especially those related to the capital cost and operating cost. Those costs depend on reflux ratio, number of stages, number of trays, reflux ratio, size of the distillation column vessel, feed flow rate, the composition of the products required, and the utilities needed by reboiler and condenser (Edgar, Himmelblau, & Lasdon, 2001).

Increasing reflux ratio increases required condenser heat duty but reduces the number of stages required thus reducing the capital cost as well as the operating cost. Thus, the engineer must find the optimal value for the reflux ratio. Total reflux happens when all condensate is returned to the column as reflux so there will be no product taken. Total reflux requires only the minimum number of stages that are theoretically necessary to achieve the separation. Total reflux is usually done at start-up commission and column testing. The minimum reflux ratio is the reflux ratio required to achieve the

specified separation at a certain number of stages. For practical purposes, optimum

reflux ratio will lie between total reflux and minimum reflux ratio.
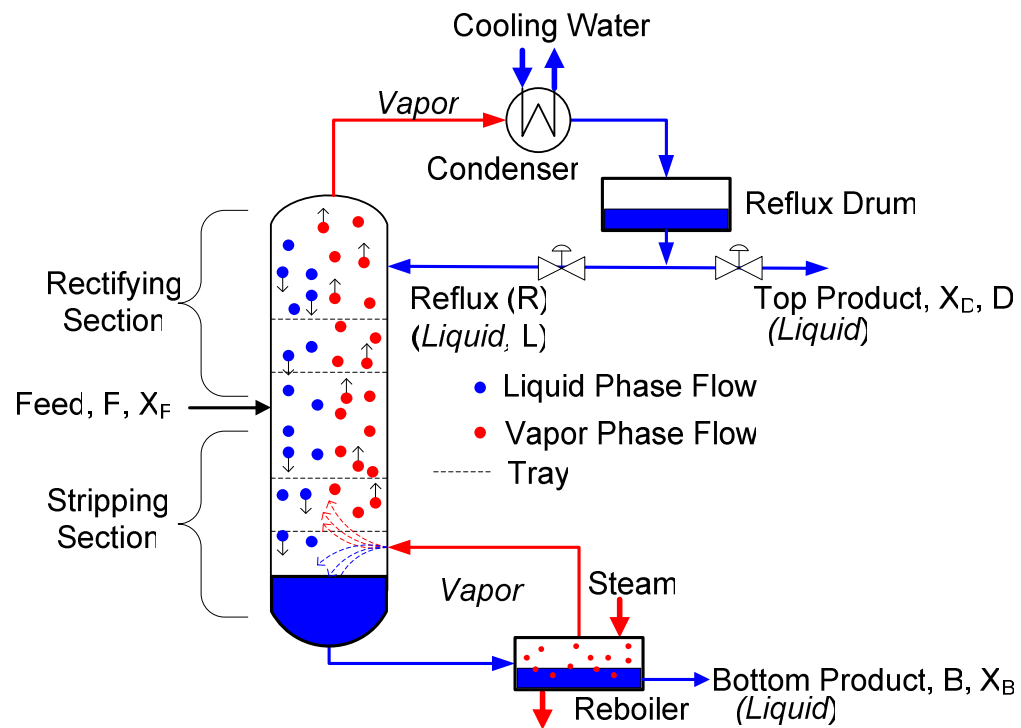
Fig. 3.2. Distillation column

Reflux ratio (R) (Sinnot, 1996) and minimum reflux ratio (Rm) (Eduljee, 1975)

are shown in Equations (3.2) and (3.3):

$$R = \frac{Flow\ returned\ as\ reflux}{flow\ of\ top\ product\ taken\ off} = \frac{L}{D} \qquad (3.2)$$

$$R_m = \frac{\left(\dfrac{X_D}{X_F}\right) - \dfrac{\alpha\left(1 - X_D\right)}{\left(1 - X_f\right)}}{\alpha - 1} \tag{3.3}$$

with X_D as mol fraction of specified product in distillate stream, X_V as mol fraction of specified product in feed stream, R_m as the minimum reflux ratio, L as the flow rate of the liquid back into column for reflux, D as distillate to product, and α as relative volatility. Physical definition of the symbol can also be seen in Figure 3.2.

The expression of reflux ratio, number of stages (N) and minimum number of stages $\left(N_m\right)$ are shown in Equations (3.4) and (3.5) (Edgar, Himmelblaue, & Lasdon, 2001):

$$\frac{\left(N - N_m\right)}{N + 1} = 0.75\left[1 - \left(\frac{\left(R - R_m\right)}{R + 1}\right)^{0.5668}\right] \tag{3.4}$$

$$N_m = \frac{\ln\left(\dfrac{X_D}{1 - X_D} \times \dfrac{1 - X_B}{X_B}\right)}{\ln \alpha} \tag{3.5}$$

with α = relative volatility.

3.3.1.1 The Diameter and the Height of the Column

The tower diameter is designed to avoid flooding when the liquid is filling the tower due to too high vapor velocity. Therefore, to calculate the diameter, the flooding velocity must be determined by Equations (3.7) and (3.8) (Peters & Timmerhaus, 1991). Then the diameter is determined by using Equation (3.6) (Peters & Timmerhaus, 1991).

$$Di = \left[\frac{4\,V_t}{u_f \times \rho_G \times \pi}\right]^{0.5} \tag{3.6}$$

$$\rho_G = \left(\frac{\dfrac{Po - 14.7}{14.7}}{(0.002866 \times T)}\right) \times MW \tag{3.7}$$

$$u_f = K_1 \sqrt{\frac{\rho_L - \rho_v}{\rho_v}} \tag{3.8}$$

with :

u_f = flooding vapor velocity, m/s, based on the total cross-sectional area.

K_1 = empirical constant [=] $\dfrac{ft}{s}$

ρ_L = liquid density [=] $\dfrac{lb}{ft^3}$

ρ_v = vapor density [=] $\dfrac{lb}{ft^3}$

T = operating temperature [=] K

MW = Molecular weight [=] $\dfrac{lb}{lbmol}$

Po = operating pressure [=] atm

Di = inside diameter [=] ft

The height of the distillation column (L) is calculated by using Equation (3.9).

$$L = tray\ spacing \times N \tag{3.9}$$

Based on the diameter and the height of the column, the cost of the distillation column can be determined.

3.3.1.2 The Distillation Column f.o.b Purchase Cost Estimation

Distillation column consists of tower vessel and plates/packing. The detailed description is presented hereafter. The capital cost of the distillation column is the summation of the vessel cost and the installed plates/packing cost.

A. Vessel

Distillation column tower is a vertical pressure vessel in cylindrical form. Seider, Seader, & Lewin (2004) presented a method of intermediate complexity which is based on the weight of the shell and two 2:1 elliptical heads. The f.o.b (free on board) purchase cost (C_T) of distillation column tower includes the nozzles, the manholes, a skirt, and the internals (not plates and/or packing). The f.o.b cost is based on the platform, the ladder, the weight of the tower, the wall thickness of the shell, two heads, the tower diameter, and the tower height.

The equations are shown in Equations (3.10) – (3.13):

Towers for 9,000 lb $< W <$ 2,500,000 lb (Seider, Seader, & Lewin, 2004):

$$C_V = \exp\{7.0374 + 0.18255[\ln(W)] + 0.02297[\ln(W)]^2\} \qquad (3.10)$$

Platform and ladder are additional cost, C_{PL} and depend on inside diameter D_i (ft) and the length of the shell L (ft):

Towers with $3 < D_i < 24$ ft and $27 < L < 170$ ft (Seider, Seader, & Lewin, 2004):

$$C_{PL} = 237.1(D_i)^{0.62216}(L)^{0.80161}$$ (3.11)

The weight, W, depends on the D_i (ft) and the length of the shell L (ft). For 2:1 elliptical heads, the weight of the shell and its two heads is determined by using Equation (3.12) (Seider, Seader, & Lewin, 2004):

$$W = \pi \left(D_i + t_s \right)\left(L + 0.8 D_i \right) t_s \rho$$ (3.12)

When corrosion, wind, and earthquake are neglected and the internal pressure is greater than the external pressure (i.e., excluding vacuum operation), the wall thickness is calculated by ASME pressure-vessel code formula as shown in Equation (3.13) (Seider, Seader, & Lewin, 2004):

$$t_p = \frac{P_d D_i}{2SE - 1.2P_d}$$ (3.13)

with t_p as the wall thickness to bear up the internal pressure (inches), P_d as the internal design pressure (psig), D_i as the inner shell diameter (inches), S as the maximum allowable stress of the material at the design temperature (psi), and E as the fractional weld efficiency.

The maximum allowable stress S depends on the material of construction and the design temperature. The design temperature can be taken as the operating temperature plus 50°F. It is recommended that the design pressure be greater than the operating pressure (Seider, Seader, & Lewin, 2004). For operating pressures between 0 and 5 psig, the recommended design pressure is 10 psig. In the range of operating

pressures from 10 psig to 1,000 psig, Equation (3.14) should be used to determine design

pressure (Seider, Seader, & Lewin, 2004):

$$P_d = \exp\{0.60608 + 0.91615[\ln(P_o)] + 0.0015655[\ln(P_0)]^2\} \qquad (3.14)$$

with P_0 represents operating pressure (psig).

For operating pressures greater than 1,000 psig, the design pressure is 1.1 times the

operational pressure.

B. Plates

The cost for plates with all downcomer, C_T, is provided by Equation (3.15)

(Seider, Seader, & Lewin, 2004):

$$C_T = N_T F_{NT} F_{TT} F_{TM} C_{BT} \qquad (3.15)$$

C_{BT} is the base cost.

For Sieve Trays at CE cost index of 394 and inside diameter in the range of 2 to 16 ft,

C_{BT} is given by Equation (3.16):

$$C_{BT} = 369 \exp(0.1739D_i) \qquad (3.16)$$

N_T is the number of trays utilized in the column distillation. If N_T is greater than 20

then $F_{NT} = 1$, and if it is lesser than 20 then $F_{NT} > 1$ as given by Equation (3.17) (Seider,

Seader, & Lewin, 2004)

$$F_{NT} = \frac{2.25}{1.0414^{NT}} \qquad (3.17)$$

F_{TT} for the sieve tray is 1.0 (Seider, Seader, & Lewin, 2004). F_{TM} accounts for the correction for the material of construction and depends on the column diameter as given by Equations (3.18) – (3.22) (Seider, Seader, & Lewin, 2004):

For **Carbon Steel**:

$$F_{TM} = 1.0 \tag{3.18}$$

For **303 Stainless steel**:

$$F_{TM} = 1.189 + 0.0577 D_i \tag{3.19}$$

For **316 Stainless steel**:

$$F_{TM} = 1.401 + 0.0724 D_i \tag{3.20}$$

For **Carpenter 20CB-3**:

$$F_{TM} = 1.525 + 0.0788 D_i \tag{3.21}$$

For **Monel**:

$$F_{TM} = 2.306 + 0.1120 D_i \tag{3.22}$$

3.3.2 Reactor Design Equations

In this research we use the Plug Flow Reactor (PFR) as a case study. PFR assumes that there is no diffusion along the flow path, all materials have the same velocity as the materials advance through the length of the reactor, no longitudinal mixing along the flow path, and no radial gradient in either temperature and concentration. The performance of the reactor can be determined by using the following data:

1. The rate of reaction and the mass transfer characteristics of the reacting fluid. This determines the volume of the reactor needed to produce the specified product.

2. The constraints dictated by the reactor are set up such as the type and the geometry of the reactor. This determines the cost of the reactor and thus the economic parameter. Economic variables of reactor are type, diameter, height, design pressure, material of construction, and capacity (Edgar, Himmelblau, & Lasdon, 2001).

Conversion (X) is the measure on how far the reaction has proceeded and is in the range of 0 to 1 (100 % conversion). In optimizing a reactor, the conversion might not reach 100% conversion due to other constraints such as economic factors. For reaction with more than one reactant, the material which the conversion is based on must be specified. Conversion expression is:

$$Conversion = \frac{amount\ of\ material\ consumed}{amount\ material\ provided}$$

$$= \frac{(amount\ in\ inlet\ stream) - (amount\ in\ outlet\ stream)}{amount\ in\ inlet\ stream} \quad (3.23)$$

Generally, the independent variables are pressure, temperature, flow rate, and concentration of the feed. There is no general optimization model for reactor hence the model is developed for each specific case. For this research, Plug Flow Reactor (PFR) reactor is used with reaction of: A → B + C (gas phase), whose models are given in Equations (3.24) – (3.26) (Fogler, 2002):

- PFR design equations, rate law for A ----> B + C, and stoichiometry:

$$Volume = \frac{\pi}{4} D_i^2 L = F_{Ao} \int_0^X \frac{dX}{-r_A} \tag{3.24}$$

$$-r_A = k\, C_A \tag{3.25}$$

$$C_A = \frac{C_{Ao}(1-X)}{(1+\varepsilon\, X)} \tag{3.26}$$

with D_i as inside diameter, F_{Ao} as molar flow rate of the reactant A, X as the reactor conversion, C_A as the concentration of A in the reactor, ε as volume changes in gas phase reaction, and C_{A0} as the concentration of component A at the reactor entrance.

- Combining design equation, rate law, and stoichiometry:

$$Volume = \frac{\pi}{4} D_i^2 L = \frac{F_{Ao}}{k\, C_{Ao}} \left[(1+\varepsilon) \ln \frac{1}{1-X} - \varepsilon\, X \right] \tag{3.27}$$

3.3.2.1 The Reactor f.o.b Purchase Cost Estimation

PFR reactor is a cylindrical vessel that can be determined in the same way as that of the distillation column with several modifications, only in different orientation. The reactor is a horizontal pressure vessel in cylindrical form. The f.o.b purchase cost (C_P) of horizontal pressure vessel including the nozzles, the manholes, a skirt, and the internals (not plates and/or packing) are described by Seider, Seader, & Lewin (2004) in Equations (3.28) – (3.29):

Horizontal vessel for 1,000 lb < W < 920,000 lb (Seider, Seader, & Lewin, 2004):

$$C_V = \exp\{8.717 - 0.2330\,[\ln(W)] + 0.04333\,[\ln(W)]^2\} \tag{3.28}$$

Platform and ladder are additional cost, C_{PL} and depend on the inner diameter D_i (ft) and the length of the shell L (ft):

Horizontal vessel with $3 < D_i < 12$ ft (Seider, Seader, & Lewin, 2004):

$$C_{PL} = 1{,}580(D_i)^{0.20294} \tag{3.29}$$

W, t_p, and P_d are evaluated by Equations(3.12), (3.13), and (3.14).

Chapter III has presented the reactor-distillation column design and economic parameters. Optimization models in this research are built based on the equations in Chapter III. Before performing optimization, it is necessary to understand the theory of optimization, which is described in Chapter IV.

CHAPTER IV

OPTIMIZATION

4.1 OVERVIEW

It is one of the primary tasks of a chemical engineer to design and operate chemical processes and ensure them working faster, better, cheaper, safer and greener (El-Halwagi, 2003). During designing process, there is a correlation between technical design and economic analysis. In practice, it is very important to have an economically optimum and inherently safer design which is the best design based on technical and business performance within acceptable safety level. How do engineers incorporate those three parameters into process design while achieving the specified product(s)? Process optimization with technical performance, business performance, and safety parameters as the constraints might be a good solution. This research attempts to perform this optimization and analyze the result.

There are several methods available to solve the optimization problem, manually or computerized. This research solves the optimization problem using software LINGO$^{®}$ by LINDO Inc which is a linear and non-linear solver. Computer software offers faster and efficient calculation so that this research can focus more on the development of the mathematical models of the process evaluated and the validation of the proposed methodology. We decide to use LINGO® based on availability, simplicity, and researcher's familiarity as well.

4.2 BASIC OF OPTIMIZATION

Optimization deals with the use of efficient and effective quantitative method to find the optimal solution in the whole solution space. Optimization consists of two steps: formulating the problem and using mathematical techniques to solve it. However, as many mathematical tools are available, the formulation of the problem becomes an important task. Chemical engineers play a very important role in chemical process optimization as they have enough basic knowledge in equipment design and chemical processes. Chemical engineer must find the optimization variables that affect the process significantly as well as define the objective function criteria. The purpose of optimization is to maximize or minimize the values of a set of functions (called objective functions) subject to a variety of restrictions (called constraints) (El-Halwagi, 2003). A typical optimization problem consists of three essential parts: at least one objective function, equality equations, and inequality equations as constraint.

Edgar, Himelblau, & Lasdon (2001) presented the optimization problem in the form of:

Minimize   : $f(x)$ objective function   (a)

Subject to   : $h(x) = 0$ equality constraints   (b)

               $g(x) \geq 0$ inequality constraints (c)

With x is a vector of n variables $(x_1, x_2, x_3, x_4, ...)$, $h(x)$ is a vector of equations of dimension m_1, $g(x)$ is a vector of inequalities of dimension m_2 and the total number of constraints is $m = (m_1 + m_2)$.

For example:

Objective function: maximum conversion (X).

Equality constraint: $F_A = F_{A_0}(1 - X)$

Inequality constraint: $X \geq 0$

Edgar, Himmelblau, & Lasdon (2001) also proposed seven steps to solve optimization problems as follows:

1. Define the process variables and specific characteristics of interest by generating a list of all available variables.

2. Develop the process models by determining the optimization criteria and the objective functions in terms of variables defined in step 1 together with the coefficients.

3. Develop mathematical process or equipment models that relate the input-output variables together with the coefficients, including both equality and inequality constraints.

4. Define the type of process model (underdetermined, over-determined, unique solutions) by identifying the independent and dependent variables to obtain the number of degree of freedom. Mass balances, energy balances, empirical equations, conceptual constraints (non-negativity requirement such as conversion must be greater than zero, etc), external restriction and other physical and chemical principles are among the base knowledge in developing the model.

5. If the process model is too large and complex:

a. Divide into smaller and manageable model.

b. Simplify the objective model and the process model.

6. Apply the appropriate optimization method to the process model.

7. Cross check the answer and do the sensitivity analysis for the uncertainty with the coefficients and assumptions of the model to analyze or examine the answer.

Since this research employs computer software to solve the optimization, this chapter will also focus on the development of mathematical/optimization model of the system under evaluation. The mathematical model is developed based on the fundamental chemical and physical laws applied to the system as well as the objective function. There is no specific method on developing mathematical models, it is specific for an individual system. For example, this research is using a reactor-separator system with the total of operating and capital cost as the objective function. Based on their physical properties, reactor and separator consist of vessels. The diameters, the heights, and the constructing materials of the vessels will determine the total cost. The diameters and the heights of the vessels are calculated from the rate of reaction, the material balance, the operating temperature and operating pressure, which are based on the chemical process of the system. In addition, by incorporating the fact that safety concerns set limits on the temperature, pressure and material, conversion is in the range of 0 to 100%, and design limits the product specification, the equality and inequality constraints can be developed.

All of the equations involved will be the input for LINGO. The detail of the equation used has been presented in Chapter III. The next chapter, Chapter V, presents

the case study which shows the mathematical model for reactor-separator system developed and the solution from LINGO.

CHAPTER V

FIRE AND EXPLOSION INDEX PROGRAM DEVELOPMENT

5.1 OVERVIEW

As described previously in chapter II, F&EI seeks to quantify the process information which is related to hazards (i.e., process conditions, materials, types of equipment and other characteristics of the process) in the form of "penalties" and "credit factors". AIChE (1994) presented the F&EI manual which provides detailed procedures, descriptions, equations, graphical data, and tabular data, but not in the form of computer software. This makes the calculation even more time consuming when it is done manually. Moreover, manual calculation requires the user to have the Dow handbook at hand, limits the ability to document the F&EI calculation process, and reduces the capability to perform sensitivity analysis and multiple calculations. Therefore, the idea to automate the F&EI calculation arises.

Etowa, Amyottee, Pegg, & Khan (2002) developed a computer program to automate F&EI calculation and perform sensitivity analysis using Microsoft® Visual Basic. However, their program was not intended to determine business interruption and loss control credit factors, to conduct process unit risk analyses, to automate the sensitivity analysis, or to integrate F&EI calculation into process design and optimization framework.

F&EI program developed in this research is presented in this chapter. The ability to calculate the F&EI, to determine loss control credit factors and business interruption,

and to perform process unit risk analysis is the unique feature in this F&EI program. In addition to F&EI calculation, F&EI program provides the descriptions of each item of the penalties and the chemicals/materials databases. The ability to add chemical/material data to the databases and to calculate material factors are provided so that the user can use the program without the F&EI book at hand. Moreover, the sensitivity analyses are automated by generating charts and expressions of F&EI as a function of material inventory and pressure. The expression will be the focal point in integrating F&EI into process design and optimization framework.

Part of this research is to develop a user-friendly program based on the Dow Fire and Explosion Index 7th edition (1994 version). The programming language used is Microsoft Visual Basic$^{®}$ Application (VBA) with Microsoft$^{®}$ Excel (Excel) as the host application. All codes related to penalties, credit factors, databases, and other functions of the F&EI program are available in the Appendix: Algorithms for Microsoft$^{®}$ Visual Basic application**.**

The optimization problem could be solved by various tools. We investigate the optimization problem using LINGO$^{®}$ 8.0 software by Lindo System Inc.. LINGO$^{®}$ is employed because of its simplicity, availability, and researcher's familiarity as well. LINGO$^{®}$ is a comprehensive tool to solve linear, nonlinear, and integral optimization models faster, more easily and efficiently.

This chapter presents guidelines to use the F&EI program.

5.2 LINGO®

LINGO® is a mathematical modeling language and different from other basic programming languages such as BASIC or C ++. LINGO® is non-procedural so that the users are only to specify what they want, not how to find the solution. Therefore, LINGO® allows the user to express the model in a standard mathematical notation without additional codes or syntaxes.

5.2.1 LINGO® Syntax and Functions

There are several rules on writing problem statements in LINGO®, which are:

- It is not necessary to write the mathematical statement in a certain order. All statements are considered as the variable that must be satisfied.

- LINGO® does not differentiate small and big caps, i.e., y and Y are considered as the same variable. It handles up to 32 characters length of variables which must begin with a letter (A-Z) and allows any alphanumeric character and underscore.

- Every statement must end with a semicolon (;). This allows the user to have a long statement with more than 1 line. Example: `tp=(Pd*Di)/(25500-1.2*Pd);` can also be written as:

```
tp=(Pd*Di)/
(25500-1.2*Pd);
```

- Comment begins with exclamation point (!) and ends with semicolon (;). Comment can be more than 1 line or share lines with other LINGO® statement.

  Example:

Comments
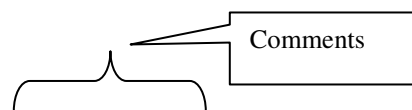
```
Cao=0.00415; ![=]lb mol/ft3;
```

LINGO® defines only two types of mathematical functions: general and trigonometric. This research employs the following LINGO® general mathematical functions:

- @EXP(X) – returns the constant e(2.718281…) to the power X.

- @LOG(X) – returns the natural logarithm of the function X.

- MIN=f(X) or MAX=f(X) - to find maximum or minimum value of the objective function statement.

After all models are submitted to LINGO®, LINGO® will provide the result in a new opened-window. All LINGO® models and their solutions applied in this research are available at Appendix B.

5.3 SYNTAX USED IN MICROSOFT® VISUAL BASIC APPLICATION (VBA)

VBA file is not an executed file, thus it must be open in any Microsoft® Office™. In this research, the host application is Microsoft® Excel, thus the user must open Microsoft® Excel to run the F&EI program. Based on the written text, tabular data, graphs, and expressions in the Dow book, most of the safety parameters, penalties, and credit factors on the F&EI can be described as *If…Then* statements, hence algorithms for the F&EI are prepared in that form. The following are several things that must be understood before the algorithm can be written:

1. Function Procedures

Function procedures are applied to create functions with named arguments, optional arguments, and specific data type results that are compatible to Microsoft® Excel. It is a VBA procedure that returns a result. Harris (1997) present that the user simply specifies the arguments the function uses, the actions to be performed, and the value that the function returns and describes the general syntax for a function as the following:

Function *name* ([*arglist*])

'VBA Statements

[*name = expression*]

End Function

Here *name* denotes the name of the function; *arglist* is the argument list of the function (several *arglist* must be separated with comma) and *name=expression* is the function assignment which tells VBA what value the function should return. The function procedure begins with the keyword **Function** followed by the function's name and ends with **End Function** keyword.

2. Variable Constant Data Type

- String Constant

   It is a non-numeric constant and must be enclosed in double quote marks (" "). A blank string constant is identified by two question marks together with nothing in between: "".

- Boolean Constant

  There are only two Boolean constants: *true* and *false*.

- Numeric Constant

  This consists only of the number 0 through 9 with no symbols or characters.

3. Decision Making Commands

   Decision making command is the VBA capability to choose between two alternatives of procedures based on whether or not the condition is satisfied. For choosing between branches of decisions, the general VBA syntax is:

   If *Condition1* Then
   > *Statement1*
   ElseIf *Condition2* Then
   > *Statement2*
   Else
   > S*tatement3*
   End If

   The conditions represent any logical expression and statements represent the consequences when the conditions are true. VBA executes all conditions according to the order. For the syntax given, if the logical expression represented by *condition1* is true then VBA executes *statement1*. However, if the logical expression represented by *condition1* is false then VBA immediately checks *condition2* without considering *statement1*, and so on. Every decision making command begins with **If….Then** keyword and ends with **End If** keyword.

4. *User-Defined Functions*

In the VBA, the user can expand the collection of the built-in worksheet functions in Excel. Excel will recognize it as *user-defined functions* which are the function procedures stored as worksheet functions in Excel. The *user-defined functions* are named by the user and contain any guidelines, arguments, and restrictions defined by the user. The codes for the function procedure combined with decision making command for exothermic chemical reaction penalty on F&EI is shown in Figure 5.1

```
Function PenaltyExotherm(ByVal dtype As String) As Double
If dtype = 1 Then
    PenaltyExotherm = 0.3
ElseIf dtype = 2 Then
    PenaltyExotherm = 0.5
ElseIf dtype = 3 Then
    PenaltyExotherm = 0.75
ElseIf dtype = 4 Then
    PenaltyExotherm = 1
ElseIf dtype = 5 Then
    PenaltyExotherm = 1
ElseIf dtype = 6 Then
    PenaltyExotherm = 1.25
End If
End Function
```

Fig. 5.1. Example: Syntax for exothermic chemical reaction penalty

Excel will recognize *PenaltyExotherm* as name of the user-defined function. To access the *PenaltyExotherm* in Excel, the function name and its arguments are introduced as a formula in a worksheet cell the same way the user would enter any input to any Excel's built-in functions. If the user does not remember the name of the function, the function can be found in *user-defined functions* organized under Excel's *insert - function* dialog, as shown in Figure 5.2.
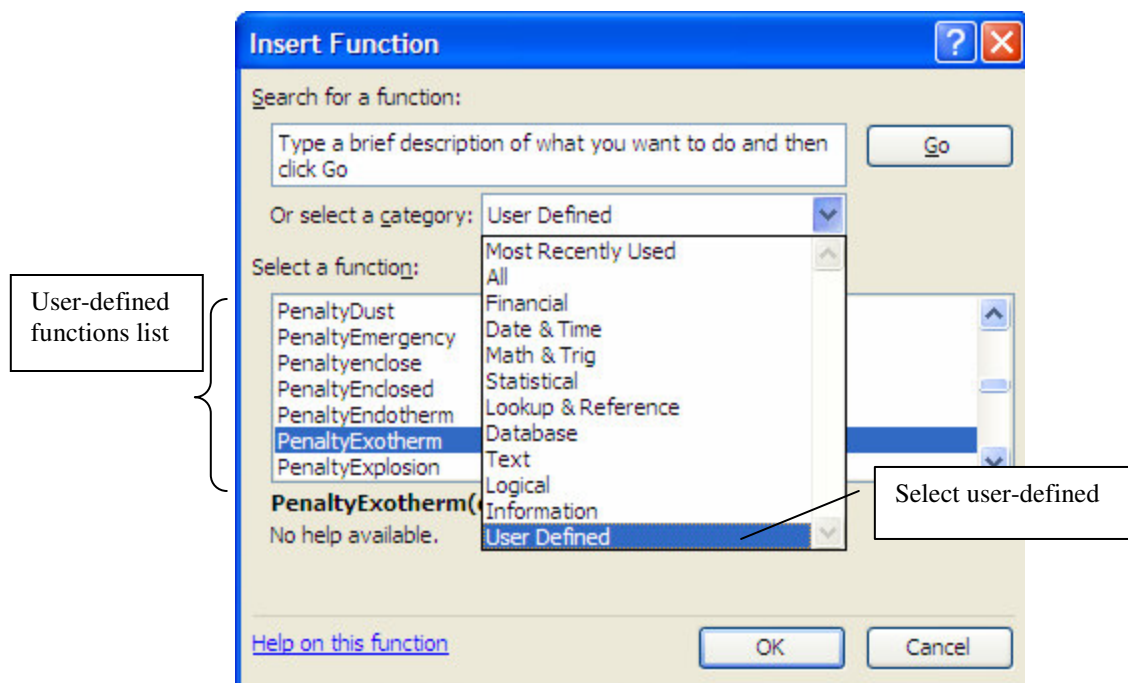
Fig. 5.2. *User-defined functions* **in Microsoft Excel (Adapted from Microsoft Excel)**

5. Creating List Box

List Box displays a list of values/statements that the user can select from. The list boxes are arranged to allow the user to select only one single value from several

available values/statements. As shown in Figure 5.3, VBA recognizes each value/statement as a sequenced number. So, the first row of value/statement is represented as 1, the second row value/statement is represented as 2, and so on.
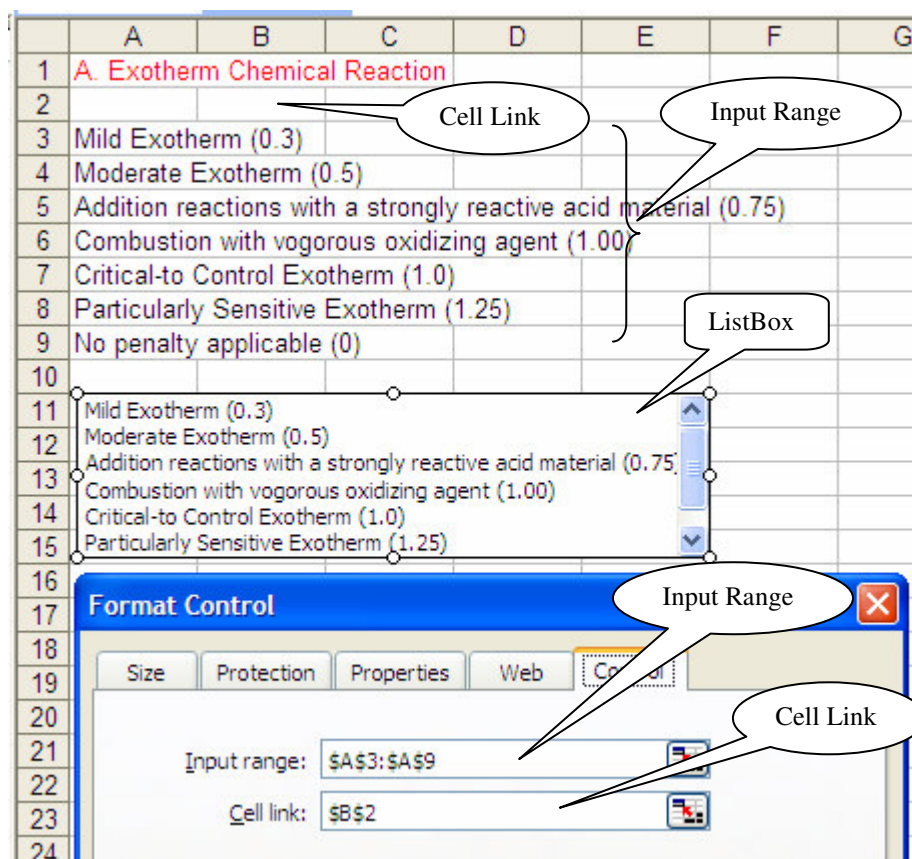
Fig. 5.3. Example of List Box for exothermic chemical reaction (Adapted from Microsoft Excel)

The user assigns a cell for each input and output by doing right click while the arrow is on the List Box and then selects format control button. In Figure 5.3, the input range is A3 to A9. If the user selects "moderate exotherm" which is the 2nd row of value/statement, then cell B2 (Cell link) will be filled by a number "2". This number is

an input to the user-defined function that was described on the section 3- *User-Defined Functions*. This research employs not only the List Box, but also Check Box and Option Box. The procedure for developing Check Box and Option Box are the same as the one for List Box.

6. Check Box

Check Box is a square box with checkmark when selected and is not for mutually exclusive procedures. Hence, the user can select more than one statement. The output of CheckBox is in the form of true/false statement which appears on the cell link assigned by the user and will be the input for the user-defined function. Figure 5.4 shows an example of CheckBox built for this research.

Fig. 5.4. Example of CheckBox for operation instruction/procedure credit factor

7. Option Button.

It is a round box that is filled with black dot when selected and is mutually exclusive. Thus, the user can select only one statement. The example of an Option Button is shown in Figure 5.5.

○ LIQUIDS AND GASES FLAMMABILIITY OR COMBUSTIBILITY AND VOLATILE SOLIDS
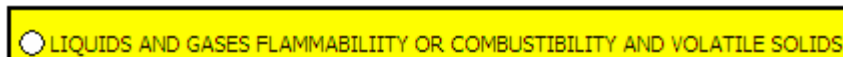
Fig. 5.5. Check box for material factor determination

5.4 GUIDELINES FOR OPERATING F&EI PROGRAM

The F&EI program has so many features that are represented by buttons. To be able to use those features, the user selects the certain buttons available in F&EI navigator. The detailed features are described in the following sections.

5.4.1 F&EI Navigator

F&EI navigator box is a house for many buttons to perform other functions in F&EI calculation, as shown in Figure 5.6. For example, to determine the material factors, the button *Material Factor* on the F&EI navigator must be selected. The following section will describe the features of each buttons.

- Data Input

    This button is used to verify whether the material used in the F&EI calculation is in the databases that the program provides.
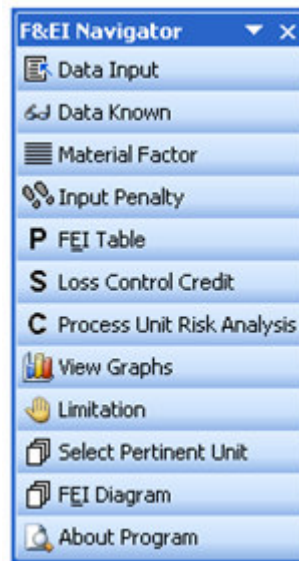
Fig. 5.6. F&EI navigator

- Data Known

  This button is selected when material data is not in the databases but available on other sources. The user submits the data to the program databases using a pop-up form that appears after clicking *Data Known* button.

- Material Factor

  This button is used only when the material data is neither listed in the database nor available on other sources. This button will lead the user to the *Material Factor Determination for Unlisted Substances* page and shows a form for calculating the material factor.

- Input Penalty

  This button will bring the user to the page where F&EI calculation is performed.

- F&EI Table

  This button is selected if the user wants to review the summary of every penalty

  submitted, the final F&EI value, and the sensitivity analysis form.

- Loss Control Credit

  This button leads to the submission form for loss control credit factors.

- Process Unit Risk Analysis

  This button allows the user to determine the business interruption.

- View Graphic

  This button takes the user to the chart of F&EI versus operating pressure and the

  amount of the hazardous material along with their equations.

- Limitation

  This button shows the limitations of the F&EI method and program.

- Select pertinent Unit

  This button provides guidance on how to select the pertinent unit used in F&EI

  calculation.

- F&EI Diagram

  This button shows the procedure of F&EI calculation diagram.

- About the Program

  This button provides important information about the program.

5.4.2 Material Factor Determination

As illustrated in chapter II, Material factor represents the intrinsic rate of potential energy release caused by fire or explosion produced from combustion or chemical reaction. It is the basic starting point of the F&EI calculation and plays a critical role in the magnitude of the F&EI. MF is obtained from reactivity value (N_R) and flammability value (N_F). The material factor determination is demonstrated in the next sections.

5.4.2.1 Material Data Available in the F&EI Program Databases

The F&EI program provides chemical databases for more than 250 chemicals/materials and allows the user to select it from process data from *listed data ListBox*. When the material data is available in the F&EI program databases, the user is permitted to have up to four chemicals/materials in the process unit under evaluation. As mentioned in Chapter II, the program selects the chemical with the highest material factor (MF) as the basis for material factor. The *Process Data for Listed Data ListBox* is shown in Figure 5.7.

5.4.2.2 Known Data

It is possible that the material used in process unit evaluated is not available in the databases. If the data is available in any other sources, the program allows the user to input the data into the F&EI program database. Select *Data Known* button on *F&EI*

navigator then the page contained the *Data Input* form appears and permits the user to

input the known-data by selecting *Store* button. *Data Input* form is shown in Figure 5.8.

Fig. 5.7. The *Process data for listed data ListBox*

5.4.2.3 Material Data Unknown

When the material data is unknown, the user can determine it by using the material

factor determination feature in the F&EI program. The material factor depends on

reactivity value N_R and flammability value N_F (liquid, solid and gas) or dust class St (for

combustible dust or mists) which are available on *Material Factor Determination for*

Unlisted Substances page.

KNOWN DATA

DATA INPUT

Reference	Perry's
Material	
MF	
NH	
NF	
NR	
Boiling Point (°F)	
Flash Point (°F)	
Heat of Combustion (Hc, 10^3 btu/lb)	

Input Penalty   Store Data

Fig. 5.8. The *Data Input* form

The selection of *Material Factor* button on *F&EI navigator* will lead the user to that page. N_R for liquid, gas, dust, and combustible solids is determined by *Reactivity Value ListBox*. Then, check the *Option Box* according to the material used. Figure 5.9 shows the *Material Factor Determination for Unlisted Substances* page with combustible solid checked.

5.4.3 Fire and Explosion Index Calculation

As mentioned in Chapter II, F&EI calculation consists of sequential steps. The determination of each step is presented in the next sections. To make the penalty determination easier, the description of each option is available in the column next to the penalty form.

MATERIAL FACTOR DETERMINATION FOR UNLISTED SUBSTANCES

REACTIVITY VALUE

The Determination of reactivity value (N_R)

Materials exhibit exotherm at 302 oF < T ≤ 572 oF (1)   ▼

☐ Materials is an oxidizer

N_R :   1

○ LIQUIDS AND GASES FLAMMABILIITY OR COMBUSTIBILITY AND VOLATILE SOLIDS

The Determination of flamability value (N_F)

73 oF ≥ F.P ≤ 100 oF (3)   ▼

N_F :   3

Material Factor :   21

⦿ COMBUSTIBLE SOLIDS

The Determination of flamability value (N_F)

Non-dusting gound material, ex: polystyrene (2)   ▼

N_F :   1

Material Factor :   14

○ COMBUSTIBLE DUST OR MISTS

The Determination of Dust Class (St)

St-2 (Kst 200-300 bar m/sec) (2)   ▼

St: 2

Material Factor :   21

Fig. 5.9. The Material Factor determination for unlisted substances page

5.4.4 General Process Hazards

Selecting *Input Penalty* button will bring the user to the *Fire and Explosion Index Calculation* page which is composed of five green buttons: general process, special process hazards, process control credit factor, process unit risk analysis, and chart. To complete the F&EI calculation successfully, the user should go through each of them.

General process hazard calculation is conducted by selecting the *General Process* button then the page shown in Figure 5.10 appears and allows the user to give penalty for each *ListBox* (A-F) according to the process under evaluation.

GENERAL PROCESS HAZARDS

A **Exothermic Chemical Reactions**

No penalty applicable (0)

Penalty : 0

B **Endothermic Processes**

Endothermic process in the reactors only

Penalty : 0.2

C **Material Handling and Transfer**

NF = 3 Combustible solids (0.65)

☐ Stored in rack without in-rack sprinkler
Penalty : 0.65

D **Enclosed or Indoor Process Units**

No penalty applicable (0)

☐ Properly designed mechanical ventilation installed
Penalty : 0

Fig. 5.10. The *General Process Hazards* page

5.4.5 Special Process Hazards

The *Special Process Hazards* page is available by selecting the *Special Process Hazard* button. There are the *Special Process Hazard Penalty ListBox* (A-L) and the *Special Process Hazard Data ListBox*. Both ListBox are shown in Figure 5.11 and 5.12.

Fig. 5.11. The *Special Process Hazard Data ListBox*

Fig. 5.12. The *Special Process Hazard Penalty ListBox*

5.4.6 Process Control Credit Factor

The "process control credit factor" page, as shown in Figure 5.13, will appear upon selecting the "P*rocess Control Credit Factor"* button. This page contains three parts: Process Control Credit Factor (C_1) with A-I list box, Material Isolation Credit Factor (C_2) with A-D list box and Fire Protection Credit Factor (C_3) with A-I list box.

Fig. 5.13. The *Loss Control Credit Factor ListBox*

5.4.7 Process Unit Risk Analysis

Process Unit Risk Analysis page is accessible by clicking the *Process Unit Risk Analysis* button. This page contains process unit risk analysis data form and process unit risk analysis summary, as shown in Figure 5.14.

FIRE AND EXPLOSION INDEX CALCULATION

| General Process | Special Process Hazards | Process Control Credit Factor | Process Unit Risk Analysis | Chart |

PROCESS UNIT RISK ANALYSIS SUMMARY

PROCESS UNIT RISK ANALYSIS DATA

Original Cost	1,000,000	US $
Process Unit Hazards Factor	11.55	
Material Factor	24	
Value of Production for The Month (VPM)	5,000,000	US $
Maximum Probable Days Outage (MPDO)	#VALUE!	Days
CE Plant Cost Index	318.4	Year 1998

PROCESS UNIT RISK ANALYSIS SUMMARY

1	Fire and Explosion Index (F&EI)	277.26	
2	Radius of Exposure	232.90	ft
	Process equipment is the center of the circle using radius of exposure	84.51	m
3	The Area of Exposure	170,318.40	ft²
		22,425.02	m²

Fig. 5.14. *The Process Unit Risk Analysis Summary* **ListBox**

5.4.8 Sensitivity Analysis Chart

The data for sensitivity analysis is given by selecting *F&EI* button. The user submits various values for the pressure and the weight of material, then select the *run sensitivity* button to run sensitivity analysis. F&EI value for each data submitted will be calculated and plotted as sensitivity analysis chart. Sensitivity analysis chart is available by selecting the *View Graph* button. This page contains the sensitivity curve and the equation that represents the curve. The sensitivity analysis form and chart are shown in Figure 5.15 and Figure 5.16, respectively.
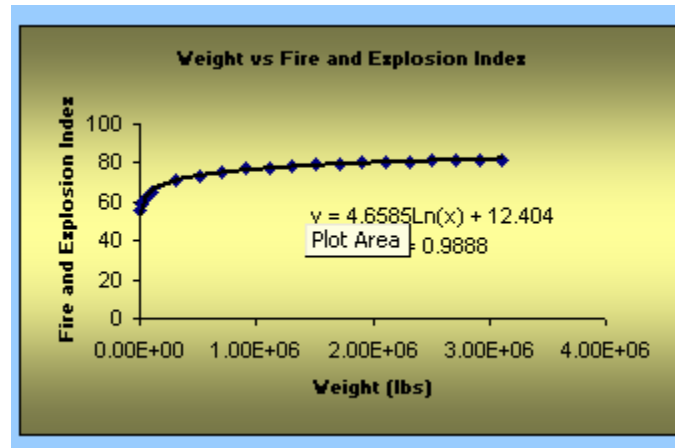
Fig. 5.15. Sensitivity chart for the weight of material and its equation

Expression of F&EI as functions of the operating pressure and the amount of material can be obtained. The expressions are ready to be integrated into process design and optimization framework. Based on process models which are presented in Chapter III and IV, we are ready to apply them into case studies. Chapter VI presents the integration of F&EI into process design and optimization with case studies.

SENSITIVITY ANALYSIS			
Weight	**FEI**	**Pressure (psig)**	**FEI**
3.11E+06	81.69871	0.5	76.90317
2.91E+06	81.53151	1.5	81.35626
2.71E+06	81.3374	2.5	81.44435
2.51E+06	81.11163	3.5	81.53314
2.31E+06	80.84821	4.5	81.62264
2.11E+06	80.53949	5.5	81.71283
1.91E+06	80.17553	6.5	81.80371
1.71E+06	79.74304	7.5	81.89528
1.51E+06	79.22381	8.5	81.98753
1.31E+06	78.59199	9.5	82.08046
1.11E+06	77.80921	10.5	82.17406
9.10E+05	76.81509	11.5	82.26833
7.10E+05	75.50664	12.5	82.36327
5.10E+05	73.68564	13.5	82.45887
3.10E+05	70.88444	14.5	82.55512
1.10E+05	65.36076	15.5	82.65203
9.50E+04	64.65038	16.5	82.74959
8.00E+04	63.84623	17.5	82.84779
6.50E+04	62.91768	18.5	82.94663
5.00E+04	61.81427	19.5	83.04611
3.50E+04	60.44187	20.5	83.14622
2.00E+04	58.58176	21.5	83.24695
5.00E+03	55.34337	22.5	83.34831
		Run Sensitivity	

Fig. 5.16. Sensitivity analysis form

CHAPTER VI

CASE STUDIES AND VALIDATION

6.1 OVERVIEW

This research presents F&EI program to generate the safety parameter expression as a function of material inventory and operating pressure and incorporate the expression into process design and optimization framework as an attempt to integrate the safety parameter integrated into design and optimization. This integration is performed according to the proposed diagram for integrating F&EI into process design and optimization as shown in Figure 6.1. The safety parameter used is Dow's Fire and Explosion Index method by AIChE (1994).

The case study and validation are performed to both the F&EI program and the proposed procedures. The validation has to confirm that the F&EI program is able to calculate the F&EI value according to the method presented by AIChE (1994) and is performed by comparing the F&EI programmed-calculation value with published F&EI value for the three case studies. Once the F&EI program is valid to be used, then it is ready to be employed to the case study of reactor-separator system.

The validation of the proposed procedures are carried out in order to make sure that integrating Dow's Fire and Explosion Index (F&EI) as a safety parameter into process design and optimization will bring benefit without sacrificing the specified economic and design parameters. In addition, the validation shows how to integrate the

F&EI, what data should be used and what kind of useful output should be getting. The remainder of this of this chapter presents the case study and validation.
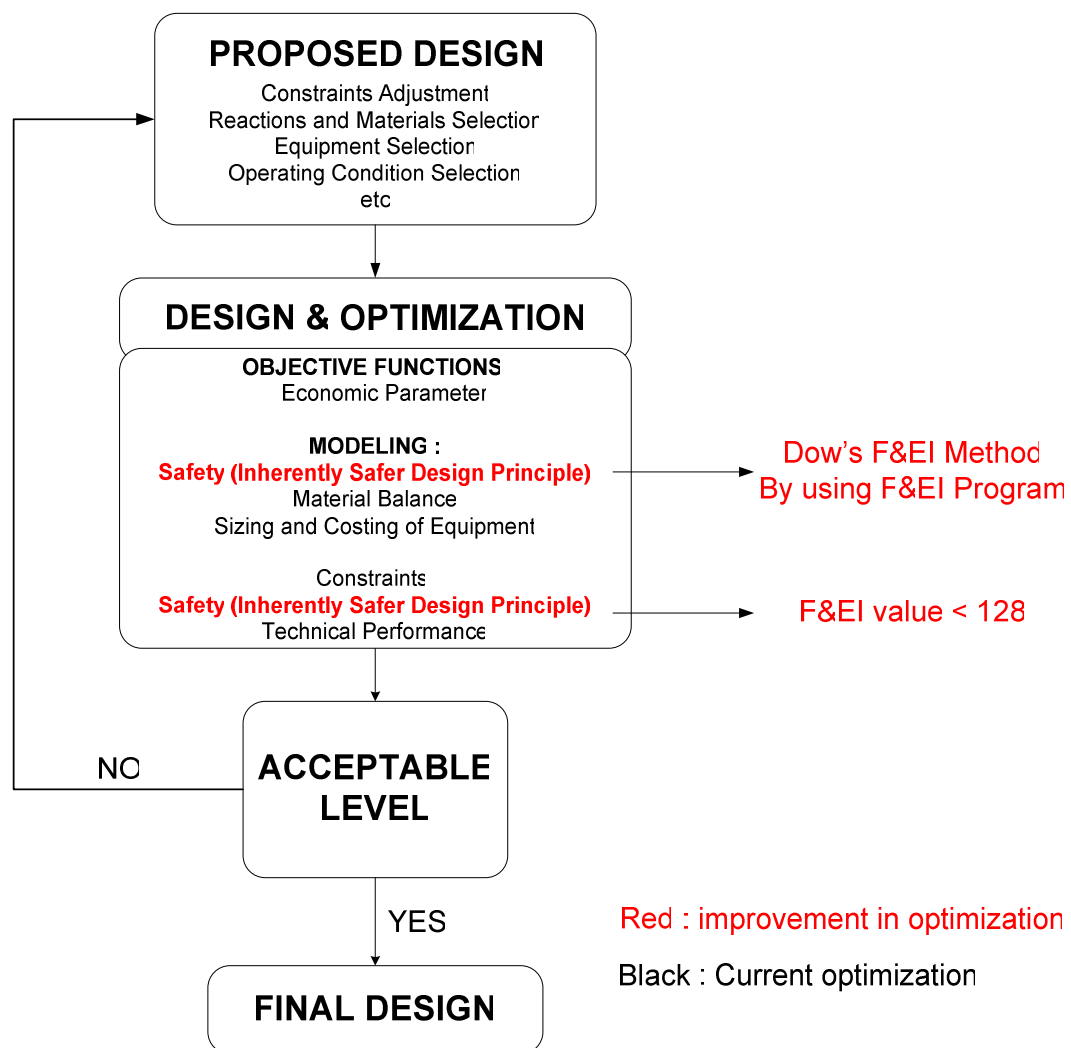
Fig. 6.1. Proposed procedure for integrating safety into process design and optimization to achieve inherently safer design

6.2 F&EI PROGRAM VALIDATION

The case study used are the calculation of F&EI for the Bhopal Incident presented by Etowa, Amyottee, Pegg, & Khan (2002), the Nitric Acid Plants presented by Sinnot (1996), the installation of a new railcar tank unloading facility presented by Crowl & Louvar (2002), and the ammonia synthesis reactor presented by Gupta, Khemani, & Mannan (2003). Etowa, Amyottee, Pegg, & Khan (2002) calculated the F&EI for Bhopal by using their own F&EI program to calculate F&EI value. However, their program is not able to calculate the business interruption, to perform sensitivity analysis and to generate the F&EI expression as a function of material inventory and operating pressure. Moreover, all of the case studies only present the F&EI value except the one by Gupta, Khemani, & Mannan (2003). Therefore, the comparison of F&EI value is performed on the first three of the case study while the comparison of the loss control credit factor and process unit risk analysis are performed to the fourth case study.

The sensitivity analysis is confirmed by changing the value of both material inventory and operating pressure in the special process hazards section of F&EI manually. Then see whether the sensitivity analysis given by F&EI program will give the same results as in the manual attempt. The safety expression as the functions of the material inventory and operating pressure are generated by F&EI program through sensitivity analysis and least square method performed by MS Excel. MS Excel has been proved to give an accurate result. Hence, once the F&EI program including sensitivity analysis is validated by case studies, then the expressions are validated as well. The demonstration of F&EI program on case studies is shown in the next section.

6.2.1 Case Study 1: Bhopal Incident by Etowa, Amyottee, Pegg, & Khan (2002)

6.2.1.1 Problem Statement

The problem statement and data are given by Etowa, Amyottee, Pegg, & Khan (2002). The name of the equipment involved was tank 610 which was a horizontal tank with 2.44 m in diameter and 12.20 m long. The F&EI calculation is performed for tank 610 at normal operation. Listed are the data used in F&EI calculation given by Etowa, Amyottee, Pegg, & Khan (2002).

Data used:

- MIC in the tank is flammable liquid

- MIC reacts exothermically with water

- MIC is transferred from tank 610 to the process area continuously using pump with power more than 75 hp.

- Minor leaks on joints and flanges in the unit might occur due to corrosion which ranges from 0.127-0.254 mm/year.

- Operating temperature is 20 $^\circ$C.

- Operating Pressure is 138.2 kPa

- Relief Pressure is 284 kPa.

6.2.1.2 F&EI Program Calculation

Based on the data above, the F&EI value is calculated using F&EI program. The comparison of the results is shown in Table 6.1.

Table 6.1 The comparison of results by Etowa, Amyotte, Pegg, & Khan (2002) and by F&EI program

Data	Etowa, Amyotte, Pegg, & Khan (2002)	By F&EI Program
F_1	1.8	1.85
F_2	4.4	4.5
F_3	8.2 (7.92)	8.3
F&EI	238 (230)	241.7
Degree of Hazards	Severe	Severe

Table 6.1 shows some differences occur due to calculation error or undefined data. For example, F_3 calculated by Etowa, Amyotte, Pegg, & Khan (2002) is F_1 times F_2 so that F_3 must be 7.92 instead of 8.2. This results a different F&EI value. Other example is F_1 value. While it is possible for material handling/transfer section to receive the penalty of 0.85, the penalty based on the data given by Etowa, Amyotte, Pegg, & Khan (2002) should be 0.85. In that case, F_1 should be 1.85 and not 1.80. The last example is the F_3 where the difference came from pressure penalty section. To obtain the F_3 equal to 4.4, the adjustment for pressure penalty must be 0.7 which is applied only for highly viscous material. On the other hand, Etowa, Amyotte, Pegg, & Khan (2002) gave the liquid property not as highly viscous material but as flammable liquids.

However, all F&EI penalties are within a certain ranges defined by AIChE (1994) so that any value can be used as penalty as long as it is in the specified ranges. To accommodate the need for submitting values that is not available in the *ListBox*, F&EI program provides the user the ability to input the penalty according to their judgment. In

this case study, this ability enables the F&EI value calculated by F&EI program to be similar to the one by calculated Etowa, Amyotte, Pegg, & Khan (2002).

6.2.2 Case Study 2: The Nitric Acid Plants by Sinnot (1996)

6.2.2.1 Problem Statement

F&EI calculation for Nitric acid plants had been presented by Sinnot (1996) according to the block diagram shown in Figure 6.2.
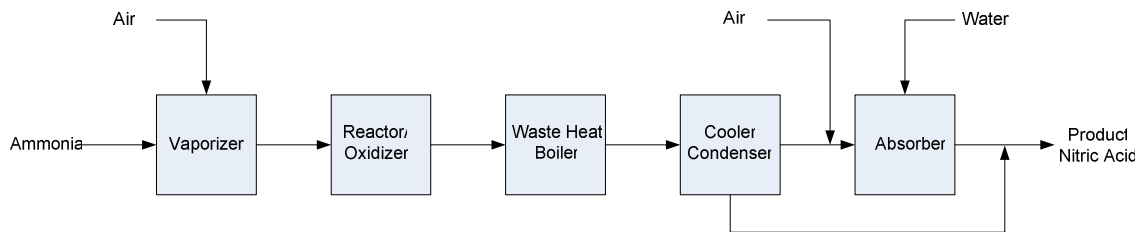
Fig. 6.2. The production of nitric acid from the oxidation of ammonia (adapted from Sinnot, 1996)

The detailed data also presented by (Sinnot, 1996):

- Unit under evaluation: Whole plant. It means that all units as a whole without separate areas and not considering main storages. Although F&EI generally performed for each pertinent unit, it is possible to consider all plant units as one pertinent unit. It is allowed only if there are no separate areas between the units and no roots of incidents for particular equipment analysis is needed.

- The largest quantity of ammonia is in Vaporizer which contains 1,100 lbs in liquid phase.

- Adequate access and drainage system are provided.

- Operating pressure is 103 psig.

- Relief valve is operated at 20 % above operating pressure.

- Corrosion due to nitric oxide fumes occurs.

- Large turbines and compressors are employed.

6.2.2.2 F&EI Program Calculation

Based on the data above, the F&EI value is calculated using F&EI program. Table 6.2 shows the comparison of the results.

Table 6.2 The comparison of results by Sinnot (1996) and by F&EI program

Data	By Sinnot (1996)	By F&EI Program
F_1	1.5	1.5
F_2	3.45	3.44
F_3	5.2	5.2
F&EI	21	21
Degree of Hazards	Light	Light

There is slightly difference but can be ignored. This results show that the F&EI program is able to calculate F&EI value for this case study.

6.2.3. Case Study 3: Ammonia Synthesis Reactor

6.2.3.1 Problem Statement

The calculation of F&EI value, process control credit factor, and process unit risk analysis for ammonia synthesis reactor have been presented by Gupta, Khemani, & Mannan (2003). They offered several penalties, credit factor and other data needed as the following:

- The material under evaluation is hydrogen.

- For general process hazards, the exothermic chemical reaction section receives the penalty of 0.30 and the access section receives the penalty of 0.20. Other sections are not applicable. Therefore, the total general process hazards factor (F_1) is 1.50.

- For special process hazards, process upset or purge failure receives the penalty of 0.30, the always in flammable range section receives the penalty of 0.80, the pressure section receives the penalty of 0.93, and corrosion and erosion section receives the penalty of 0.10. Therefore, the total special hazard factor (F_2) is 5.13

- The total process unit hazards factor (F_3) is 7.7 and the F&EI value is 161.7

- For process control credit factor (C_1), emergency power, cooling, explosion control, emergency shutdown, computer control, reactive chemical review and other process hazards analysis section receive the penalty of 0.98, 0.98, 0.91, 0.98, 0.96, 0.95, and 0.95, respectively. Inert gas, operating instruction/procedures are not applicable. Then, the total of C_1 is 0.742.

- For material isolation credit factor (C_2), remote control valves, drainage, and sections receive 0.97 and 0.94, respectively. Dump/blowdown and interlock sections are not applicable. The total of C_2 is 0.9118.

- For fire protection credit factor (C_3), leak detection, structure steel, fire water supply, sprinkler system, hand extinguisher/monitors and cable protection sections receive the penalty of 0.96, 0.97, 0.96, 0.86, 0.96, and 0.96 respectively. The special system, water curtains and foam are not applicable in this case study. The total of C_3 is 0.7085.

- For process unit risk analysis, the value of area of exposure is $ 5000/m^2$.

- Escalation factor x 0.82 is 1.

6.2.3.2 F&EI Calculation with F&EI Program

Based on the data given by Gupta, Khemani, & Mannan (2003), the F&EI value, process control credit factor, and process unit risk analysis for ammonia reactor synthesis reactor are calculated using F&EI program developed in this research. The results are presented in Table 6.3.

Gupta, Khemani, & Mannan (2003) were concentrating on calculating the loss control credit factor and process unit risk analysis. The detailed process data that are needed for F&EI were not all presented thus some differences value might occur when comparing, as shown in Table 6.3. The operating pressure and pressure relief pressure were not explicitly given by Gupta, Khemani, & Mannan (2003) so that this research is

using operating pressure for ammonia production in fertilizer companies given by Shreve (1967), which is 1049 psig.

Table 6.3 The results calculated by F&EI program and by Gupta, Khemani, & Mannan (2003)

Data	By Gupta, Khemani, & Mannan (2003)	By F&EI Program
F_1	1.5	1.5
F_2	5.13	5.16
F_3	7.7	7.7
F&EI	161.7	161.7
C_1	0.742	0.742
C_2	0.9118	0.9118
C_3	0.7085	0.7074
LCCF	0.4793 (+ 0.15 %)	0.4786
Radius of Exposure (m)	41.4	41.40
Damage Factor	0.83	0.83
MPDO (Days)	86.15	85.94
Business Interuption ($ MM)	201.017	200.516 (-0.25 %)

The pressure relief pressure has to be higher than operating pressure and is assumed as 1550 psig in this research. This results different penalty for pressure value as big as 0.03. Thus, the F&EI and other value will be different.

6.2.3.3 Sensitivity Analysis

The sensitivity analysis is also done to the case study. Manual calculation of F&EI calculation is performed at several different values of material inventory and operating pressure. Based on these values, the graph of F&EI versus material inventory

and of F&EI versus operating pressure will be generated using least squared method by MS Excel thus the expression represent the graph will be presented.

Random sample of material inventory are taken and then submitted manually as an input into the F&EI program. The results compared to the one calculated by F&EI program through its sensitivity analysis features are shown in Tables 6.4 and 6.5. The red-colored on the table shows the sample used in the manual calculation.

Table 6.4 F&EI value, inventory = 24,000 lbs, pressure relief = 1550 psig, 400 psig < operating pressure < 1500 psig

Pressure (psig)	FEI
1500	169.5
1450	169.5
1400	169.5
1350	169.5
1300	169.5
1250	169.5
1200	169.5
1150	169.5
1100	169.5
1050	169.5
1000	169.5
950	168.8
900	167.7
850	166.7
800	165.7
750	164.6
700	163.4
650	162.2
600	160.9
550	159.4
500	157.9
450	156.3
400	154.5

Inventory = 24,000 lbs	
P_R = 1550 psig	
Operating pressure (psig)	F&EI by Manual Calculation
1500	169.5
1200	169.5
900	169.5
800	167.7
600	160.9
500	157.9
400	154.5

Table 6.5 F&EI value, 14,000 lbs < inventory < 58,000 lbs, pressure relief = 1550 psig, operating pressure = 1469 psig

Inventory	FEI
1.40E+04	158.5
1.60E+04	161.4
1.80E+04	163.9
2.00E+04	166.0
2.20E+04	167.9
2.40E+04	169.5
2.60E+04	171.0
2.80E+04	172.3
3.00E+04	173.5
3.20E+04	174.5
3.40E+04	175.5
3.60E+04	176.4
3.80E+04	177.2
4.00E+04	178.0
4.20E+04	178.7
4.40E+04	179.3
4.60E+04	179.9
4.80E+04	180.5
5.00E+04	181.0
5.20E+04	181.5
5.40E+04	182.0
5.60E+04	182.4
5.80E+04	182.8

P_o = 1469 psig	
P_R =1550 psig	
Inventory (lbs)	**F&EI by Manual Calculation**
14000	158.5
16000	161.4
24000	169.5
34000	175.5
40000	177.8
46000	179.9
50000	181

Figure 6.3 shows the graph represent the sensitivity analysis and expression for both F&EI as a function of material inventory and operating pressure which are:

F&EI value = 16.776 ln (material inventory) – 0.1696

F&EI value = 2E-5 (operating pressure)^2 + 0.0538 (operating pressure) + 136.41
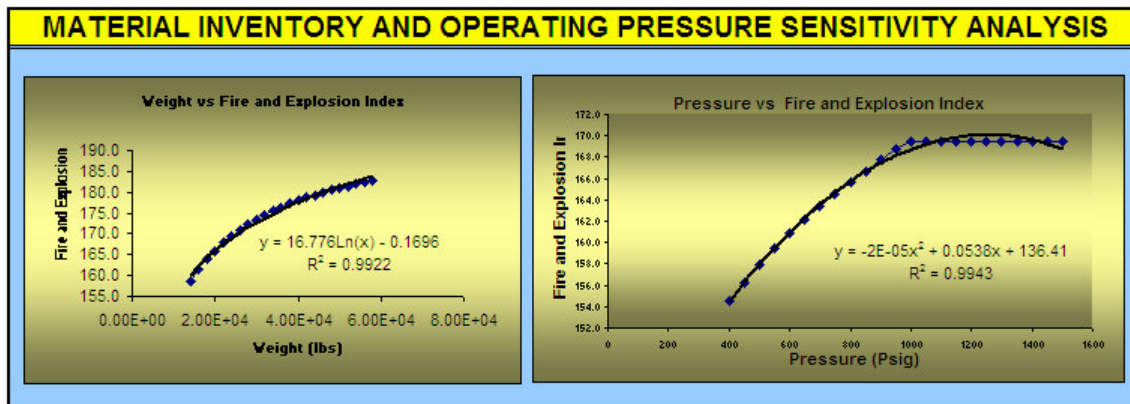
Fig. 6.3. Sensitivity analysis for operating pressure and material inventory.

6.2.4 Case Study 3: The Installation of a New Railcar Tank Unloading Facility

6.2.4.1 Problem Statement

This case study is adapted from Crowl & Louvar (2002). The data are:

- A new railcar tank unloading facility will unload 25,000 gal of either butadiene or cyclohexane.

- The system is prepared with an emergency shutdown system with remotely operated block valves.

- Inert gas is provided at the pressure of 40 psig and the pressure relief system is prepared to handle pressure of 75 psig.

- The unloading procedure instruction and reactive chemical review are available and has been reviewed by corporate technical staff.

- Combustible gas detector and a deluge system with excellent water supply are installed at unloading site.

- Diking is surrounding three sides of the facility and directs the spill to a covered impounding area.

Crowl & Louvar (2002) has performed the F&EI calculation for this system. F&EI program will calculate the F&EI value which will then be compared to the results by Crowl & Louvar (2002).

6.2.4.2 F&EI Program Calculation and Results

Based on the data above, the F&EI value is calculated by F&EI program. The results are shown in Table 6.4.

Table 6.6 The results given by Crowl & Louvar (2002) and by F&EI program

Data	By Crowl & Louvar (2002)	By F&EI Program
F_1	1.5	1.5
F_2	2.94 (+ 1 %)	2.91
F_3	4.41 (+1.1 %)	4.36
F&EI	106 (+ 1.3 %)	104.6
Degree of Hazards	Intermediate	Intermediate
Radius of Exposure (ft)	90 (+2.3 %)	87.89

6.3 VERIFICATION OF F&EI PROGRAM

After performing four F&EI calculation, one loss control credit factor and process unit risk analysis, and comparing them to the published F&EI results, the argument whether the F&EI program is reliable are going to be presented in the following.

- From the first case study, several differences occurred. Considering the cause of the differences and by comparing the results, the F&EI program has done a good job in estimating F&EI value.

- From the second case study by Sinnot (1996), the F&EI program is able to calculate the F&EI value according to the methodology presented by AIChE (1994).

- As shown in Table 6.3, the F&EI value, radius of exposure, MPDO and business interruption calculated by F&EI program are different but not more than 0.5 % than one calculated by Gupta, Khemani, & Mannan (2003). Since F&EI calculation is performed as estimation this error can be negligible. Therefore, F&EI program performs a good result for this case study.

- From the three published case study, only Gupta, Khemani, & Mannan (2003) present the loss control credit factor and business calculation. However, the comparison shows that the errors are not more than 0.6 %. This small error shows that the F&EI program perform the loss control credit factor and business calculation according to AIChE (1994).

- From the fourth case study by Crowl & Louvar (2002), all data are presented explicitly thus the calculation is much easier to do. However, Crowl & Louvar (2002) only presented F&EI value and radius of exposure calculations. The errors occur are not more than 2.5 %. Considering the cause of the errors, F&EI once again able to calculate F&EI value.

- Sensitivity analysis validation shows that the F&EI program is able to calculate the F&EI for a certain range of material inventory and operating pressure when the other process conditions are held the same. Thus, the expressions generated are also valid.

In conclusion, the F&EI program is able to perform Dow's Fire and Explosion Index methodology according to AIChE (1994). In addition, the F&EI program is ready to be applied to the next case study, the reactor and distillation column system, to examine the proposed procedures of integrating safety parameter into process design and optimization. This topic will be discussed on the next section.

6.4 CASE STUDY: REACTOR-DISTILLATION COLUMN SYSTEM

As mentioned on the overview, the integration of Dow Fire and Explosion Index as a safety parameter follows the procedures proposed in this research. This procedure will be examined in order to support the argument that integrating safety into process design and optimization give benefits without necessarily violating the economic and technical parameter. Hence, the final design is optimum economic and the inherently safer design for the distillation column system.

The reader might use more or less simple system but that will not affect the concept offered by the proposed procedures. The next section describes the case study of reactor and distillation column. In addition, it is very important to notice that the data presented in this problem statement are adapted from several sources without specifically representing a certain process. The reason is that this research in

concentrating in the concept of integrating F&EI value, not in the deep calculation of F&EI where expert judgment is really needed and in optimization process which includes a lot of variables.

6.4.1 Problem Statement

The case study used is the production of A according the reaction:

$$A \rightarrow B \text{ (gas phase)}$$
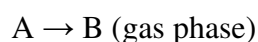
The reactor is to produce 645 million pounds of chemical B per year from chemical A. The reaction properties allow only a portion of the chemical A to be converted into chemical B. Then the output of the reactor in the form of mixture of A and B will be fed to the distillation column. Distillation column separates the chemical A and B in order to have product A in a certain number purity.

The data for the process are:

- Product is 645 million pounds of B per year.

- Pressure range is 2 - 8 atm (reactor) and 10 – 16 (Distillation column)

- Temperature is 120 F

- Reactor is isothermal and plug flow Reactor

- Feasible optimum conversion is between 40 % and 70 %.

6.4.2 Objective Functions and Optimization Model

6.4.2.1 Reactor

The objective function of this cases study is to minimize the total cost for reactor and distillation column subject to the operating pressure and the conversion.

Table 6.7 Reactor Optimization

Objective function:	Minimize Total reactor cost ($C_v + C_{pl}$)
Technical Constraints	Volume = fn (X, F_{Ao}, C_{Ao})
Economic Constraints	Cv = fn (W)
	W = fn (D, t_s, L, D_i)
	t_s = fn (P_d, D_i)
	C_{pl}= fn (D_i)
	P_d = fn (P_o)

The F&EI expressions as a function of material inventory and operating pressure generated by least squared methods on F&EI program are:

$$F \ \& \ EI = 3 \times 10^{-8} (Inventory)^2 + 0.0012 (Inventory) + 88.46$$

$$F \ \& \ EI = 0.1176 \times (pressure) + 109.8$$

6.4.2.2 Distillation Column

The expressions given by F&EI program are :

$$F \ \& \ EI = -1 \times 10^{-8} (Inventory)^2 + 0.0018 (Inventory) + 101.16$$

$$F \ \& \ EI = -5 \times 10^{-5} (pressure)^2 + 0.1072 \times (pressure) + 106.83$$

Table 6.8 Objective function and economic constraints

Objective function	Minimize Total reactor cost ($C_v + C_{pl} + C_t$)
Economic Constraints	$C_v = \text{fn } (W)$
	$W = \text{fn } (D, t_s, L, D_i)$
	$t_s = \text{fn } (Pd, D_i)$
	$C_{pl} = \text{fn } (D_i)$
	$P_d = \text{fn } (P_o)$

The equations above will be the safety constraint for the optimization. The result of the optimization for reactor-distillation column system is given in Figure 6.5.
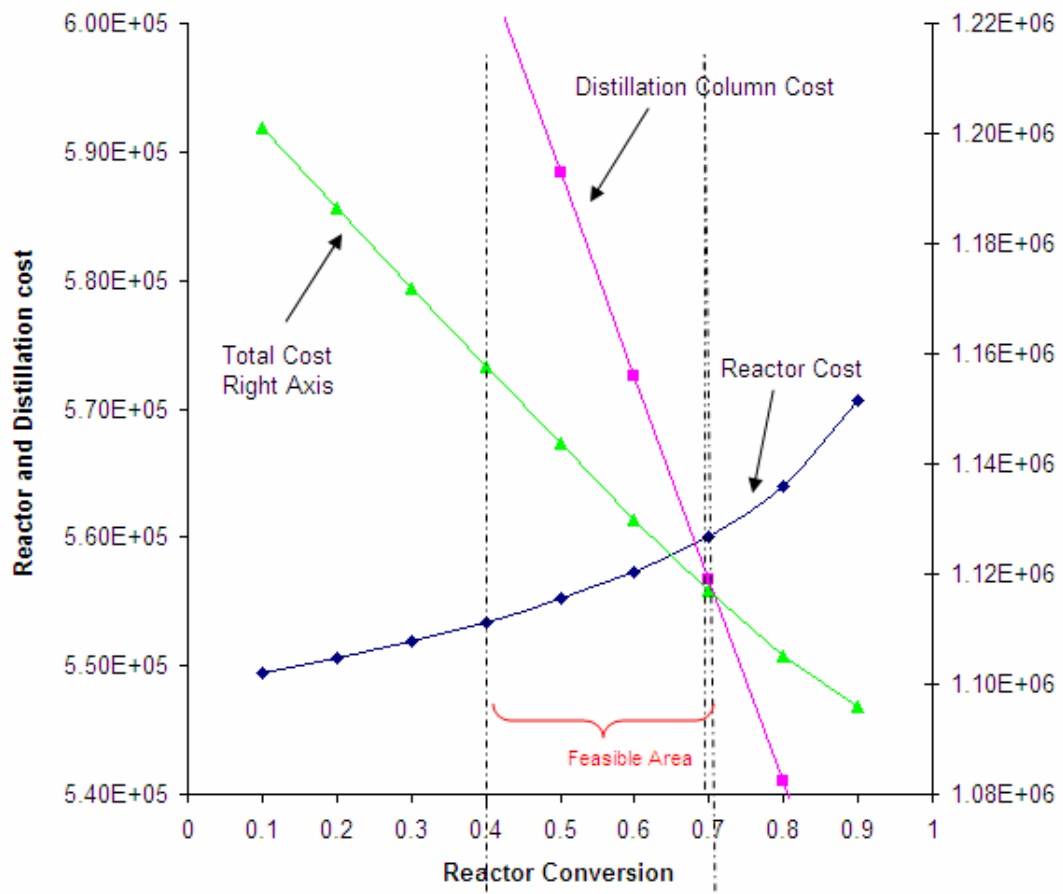
Fig. 6.4. Rector-distillation column optimization without safety constraint
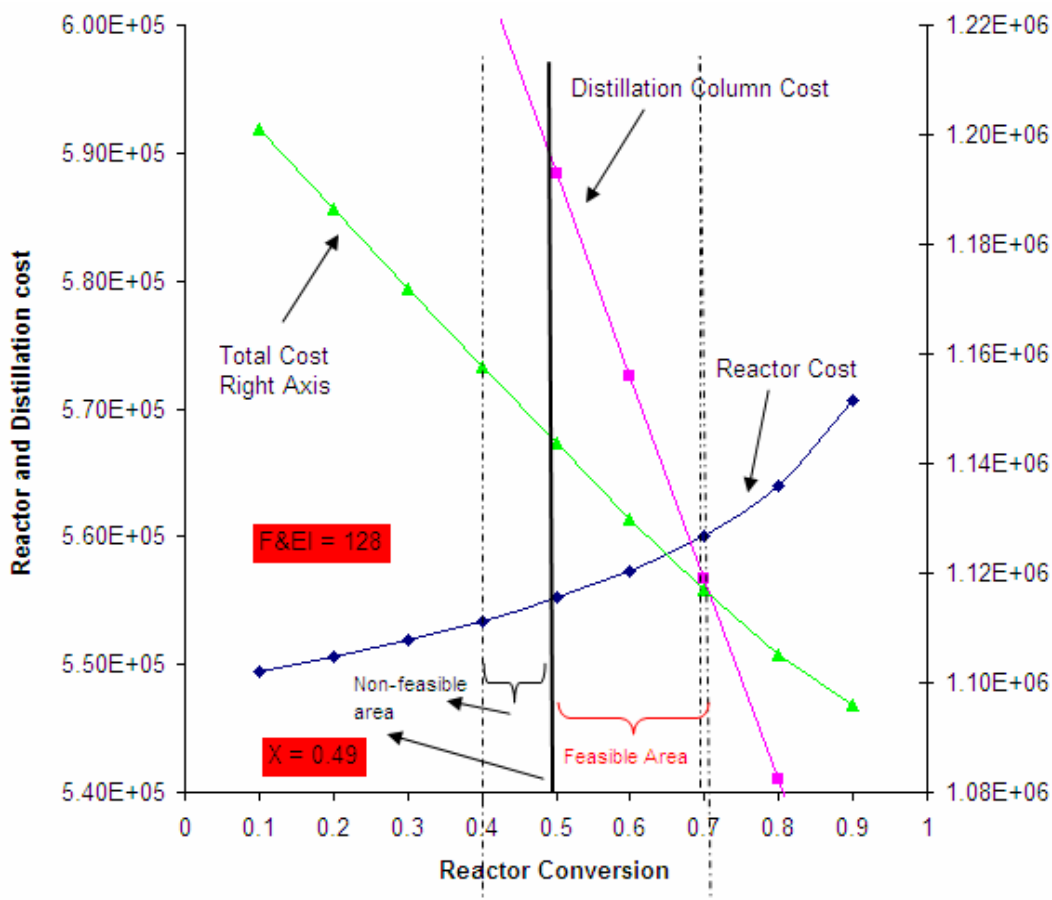
Fig. 6.5. Reactor-distillation column system with F&EI value as the safety constraint

For reactor-distillation column system, the total cost of the system is the total of the reactor cost and the distillation cost. The vertical line shows the conversion which gives the F&EI value of 128. If the safety parameter is not considered, the total cost will be available for the conversion in the range of 40 % and 70 %, as shown in Figure 6.4. However, safety parameter will not allow the process to apply those conversions since at this point the process is not inherently safer according to Dow's F&EI methodology. The

feasible range of conversion after safety parameter has been included is in the range of 49 % and 70 %, as shown in Figure 6.5.

Figure 6.5 also shows that safety parameter is employed as only one of the constraint for the optimization. It will not change any of the design value such as the cost, the reactor volume, the number of trays, etc. As a constraint, safety will only limit the feasible area for the optimization solution. Thus, if the optimization with constraint is performed, the result will be unacceptable and the designer has to adjust the constraint or the other design variables.

6.5 SUMMARY

The integration of safety parameter into process design and optimization is essential. However, there is no previous work in integrating F&EI into design and optimization. This research recommends integrating safety into design and optimization framework by using safety parameter as optimization constraint. The method used in this research is Dow's Fire and Explosion Index which is usually calculated manually.

This research automates the calculation of F&EI. The ability to calculate the F&EI, to determine loss control credit factors and business interruption, and to perform process unit risk analysis are the unique features of this F&EI program. In addition to F&EI calculation, F&EI program provides the descriptions of each item of the penalties, chemicals/materials databases, the flexibility to submit known chemical/material data to databases, and material factor calculations. Moreover, the sensitivity analyses are automated by generating charts and expressions of F&EI as a function of material

inventory and pressure. The expression will be the focal point in the process of integrating F&EI into process design and optimization framework.

The proposed procedure of integrating F&EI into process design and optimization framework is verified by applying it into process design and optimization of reactor-distillation column system. The final result is the optimum economic and inherently safer design for the reactor and distillation column system.

At F&EI value equal to 128, F&EI method will limit the amount of inventory and the operating pressure that can be used. The safety as constraint will not change the value of the variable that calculated without safety as constraint. However, it is very reasonable that in optimization process, the non-feasible area will occur. This is the reason that in the proposed procedures, when the result is not at acceptable level, the constraint (including safety parameter) must be re-arranged to get the final results.

CHAPTER VII

CONCLUSION AND FUTURE WORK

7.1 CONCLUSION

A complete fire and explosion index (F&EI) program that runs a Dow's Fire and Explosion Index has been developed and tested against four case studies. Testing against four case studies prove that the F&EI program is able to calculate the fire and explosion index, determine the loss control credit factor to reduce the F&EI value, and predict the business interruption on the process in the event of incidents, all according to Dow's fire and explosion index method presented by AIChE (1994). In addition, the F&EI program is also able to perform sensitivity analysis to generate mathematical expression of fire and explosion index as a function of material inventory and operating pressure.

The case study on reactor-distillation column system proves that the proposed procedures of integrating safety parameter (Dow's F&EI in this research) into process design and optimization framework quantitatively and systematically are really useful. The safety parameter will act more like a constraint rather than as the process variable. It will only limit the feasible area for optimization solution.

There are several contributions presented by this research:

- Developing Fire and explosion index, the most widely used and known hazard index. Texas A&M University and maybe some other school are using Dow's Fire and Explosion Index as safety parameter in their process design class.

Having the method computerized will help the student to calculate the F&EI value, loss control credit factor, business interruption, and sensitivity analysis.

- Getting safety parameter as a mathematical expression has been a problem in safety thus inhibits the integration of safety parameter into process design systematically. This research presents a simple way to generating expression from available hazard analysis which can be useful in modeling and predicting the hazard of the specific process.

- Proving that there is possibility for Dow's Fire and Explosion Index method to be integrated into process design and optimization framework while still obeys the specified technical and economic parameter.

7.2 FUTURE WORK

This work is a preliminary attempt to integrate safety parameter, not only Dow's Fire and Explosion Index, into process design and optimization framework. Therefore, there are several possibilities to extend this work:

- This research has applied the concept into reactor-distillation column system. This concept should be applied to a more complex process system to see how it works.

- This work presents F&EI program with VBA that need a host application. The F&EI program could be improved to handle more complex process and should be converted into an executed program.

- Dow's Fire and Explosion Index is not sensitive to temperature changes. Other proven safety hazards analysis with the ability to generate expression for the safety parameter, can be used and be integrated into process design and optimization. This offers wider range of application of this concept.

- Process optimization requires optimization model in the form of mathematical expression. Currently, hazards analysis methodologies quantify safety parameter without generating expression represents the safety parameter. Developing or modifying method in order to generate the safety expression give better safety parameter representation. Thus, the optimum final design can be achieved.

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APPENDIX A

ALGORITHMS FOR MICROSOFT VISUAL BASIC APPLICATION

1. General Process Hazard

A. Penalty for Exothermic Chemical Reactions

```
Function PenaltyExotherm(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyExotherm = 0.3
  ElseIf dtype = 2 Then
    PenaltyExotherm = 0.5
  ElseIf dtype = 3 Then
    PenaltyExotherm = 0.75
  ElseIf dtype = 4 Then
    PenaltyExotherm = 1
  ElseIf dtype = 5 Then
    PenaltyExotherm = 1
  ElseIf dtype = 6 Then
    PenaltyExotherm = 1.25
  End If
End Function
```

Decription for Exothermic Chemical Reactions

```
Function DetailExotherm(ByVal dtype As String) As String
  If dtype = 1 Then
    DetailExotherm = "Hydrogenation, Hydrolysis, Isomerization, Sulfonation, Neutralization"
  ElseIf dtype = 2 Then
    DetailExotherm = "Alkylation, Esterification, Addition reactions, Oxidation, Polymerization, Condensation"
```

ElseIf dtype = 3 Then

   DetailExotherm = " Reaction occuring between an strong reactive organic acid and an alcohol"

 ElseIf dtype = 4 Then

   DetailExotherm = "Vigorous oxidizing agents such as chlorates, nitric acids, hypochlorous acids and salts"

 ElseIf dtype = 5 Then

   DetailExotherm = "Reaction at which a significant fire and expoliosn potential would exist when control was lost, example: Halogenation"

 ElseIf dtype = 6 Then

   DetailExotherm = " Quite hazardous exothermic reactions such as Nitration"

 End If

End Function

B. Penalty for Endothermic Processes

Function PenaltyEndotherm(ByVal dtype As String) As Double

 If dtype = 1 Then

   PenaltyEndotherm = 0.2

 ElseIf dtype = 2 Then

   PenaltyEndotherm = 0.4

 ElseIf dtype = 3 Then

   PenaltyEndotherm = 0.4

 ElseIf dtype = 4 Then

   PenaltyEndotherm = 0.2

 ElseIf dtype = 5 Then

   PenaltyEndotherm = 0.2

 ElseIf dtype = 6 Then

   PenaltyEndotherm = 0.4

  End If

End Function

Description for Endothermic Processes

Function DetailEndotherm(ByVal dtype As String) As String

  If dtype = 1 Then

    DetailEndotherm = "This applies only to reactors"

  ElseIf dtype = 2 Then

    DetailEndotherm = "Energy provided by combustion of a solids, liquids or gaseous fuel"

  ElseIf dtype = 3 Then

    DetailEndotherm = "Heating material to remove chemically bonded water or other volatile material"

  ElseIf dtype = 4 Then

    DetailEndotherm = "Separations of ions by means of electric current"

  ElseIf dtype = 5 Then

    DetailEndotherm = "Thermal decompisition of molecules to smaller ones by use of high P, T and/or catalyst FOR ELECTRIC OR REMOTE HOT GAS HEAT"

  ElseIf dtype = 6 Then

    DetailEndotherm = "Thermal decompisition of molecules to smaller ones by use of high P, T and/or catalyst FOR DIRECT FIRED HEAT"

  End If

End Function

C. Penalty to Material Handling and Transfer

Function PenaltyInrack(ByVal IndexCombo As Byte, ByVal bChecked As Boolean) As Double

Select Case IndexCombo

  Case 1:

    PenaltyInrack = 0.5

  Case 2:

    PenaltyInrack = 0.5

  Case 3:

    PenaltyInrack = 0.85

  Case 4:

```
      PenaltyInrack = 0.65
    Case 5:
      PenaltyInrack = 0.4
    Case 6:
      PenaltyInrack = 0.25
    Case 7:
      PenaltyInrack = 0
End Select


If PenaltyInrack = 0 Then
   PenaltyInrack = 0
ElseIf bChecked = True Then
   PenaltyInrack = PenaltyInrack + 0.2


End If
End Function
```

Description to Material Handling and Transfer

```
Function DetailMaterial(ByVal dtype As String)
  If dtype = 1 Then
    DetailMaterial = "Transfer line are connected and disconnected"
  ElseIf dtype = 2 Then
    DetailMaterial = "Add air into centrifuge, batch reactors or batch mixer, whether
inerted or not"
  ElseIf dtype = 3 Then
    DetailMaterial = "Drums, cylinders, portable flexible containers and aerosol cans as
storage"
  ElseIf dtype = 4 Then
    DetailMaterial = "Foam, fiber, powder, rubber goods, styrofoam, Methocel cellulose
in dust/leak-free package"
  ElseIf dtype = 5 Then
```

    DetailMaterial = "Open<40 mm thick, coarse granular materials such as plastics pellets, rack storage, wood pallets and ground materials such as polystyrene"

  ElseIf dtype = 6 Then

    DetailMaterial = "100 < Close cup flash point < 140"

  End If

End Function

D. Penalty to Enclosed or Indoor Unit

Function Penaltyenclose(ByVal IndexCombo As Byte, ByVal bChecked As Boolean) As Double

Select Case IndexCombo

  Case 1:

    Penaltyenclose = 0.5

  Case 2:

    Penaltyenclose = 0.3

  Case 3:

    Penaltyenclose = 0.45

  Case 4:

    Penaltyenclose = 0.6

  Case 5:

    Penaltyenclose = 0.9

  Case 6:

    Penaltyenclose = 0

End Select

If Penaltyenclose = 0 Then

  Penaltyenclose = 0

ElseIf bChecked = True Then

  Penaltyenclose = Penaltyenclose * 0.5

End If

End Function

<u>Description to Enclosed or Indoor Unit</u>

```
Function DetailEnclosed(ByVal dtype As String)
  If dtype = 4 Then
    DetailEnclosed = "Can be applied to LPG"
   ElseIf dtype = 5 Then
    DetailEnclosed = "Can be applied to LPG"
   Else
    DetailEnclosed = ""
  End If
End Function
```

<u>E. Penalty to Access</u>

```
Function PenaltyAccess(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyAccess = 0.35
  ElseIf dtype = 2 Then
    PenaltyAccess = 0.35
  ElseIf dtype = 3 Then
    PenaltyAccess = 0.2
  End If
End Function
```

<u>F. Penalty to Drainage and Spills Control</u>

```
Function PenaltyDrainage(ByVal dtype As Double) As Double
  If dtype = 1 Then
    PenaltyDrainage = 0.5
  ElseIf dtype = 2 Then
   PenaltyDrainage = 0.5
  ElseIf dtype = 3 Then
   PenaltyDrainage = 0
```

    End If

End Function

2. SPECIAL PROCESS HAZARDS

Special Process Hazards Data

Amount 1

Function Material(ByVal dtype As String) As String

  If (0 <= dtype And dtype < 1000000000) Then

    Material = "The amount of material in process units"

  Else

    Material = ""

  End If

End Function

Amount 2

Function Materialconnected(ByVal dtype As String) As String

  If (0 <= dtype And dtype < 1000000000) Then

    Materialconnected = "The amount of material in the largest connected units. If the connected unit can be isolated by closure valves operable from remote location in times of emergency is removed from consideration"

  ElseIf dtype = "" Then

    Materialconnected = ""

  End If

End Function

A. Penalty to Toxic Material

Function PenaltyToxic(ByVal dtype As String) As Double

  If dtype = 1 Then

    PenaltyToxic = 0

  ElseIf dtype = 2 Then

    PenaltyToxic = 0

  ElseIf dtype = 3 Then

```
   PenaltyToxic = 1
 ElseIf dtype = 4 Then
   PenaltyToxic = 2
 ElseIf dtype = 5 Then
   PenaltyToxic = 3
 ElseIf dtype = 6 Then
   PenaltyToxic = 4
 End If
 PenaltyToxic = PenaltyToxic * 0.2
End Function
```

B. Penalty to Sub-Atmospheric Pressure

```
Function PenaltySubPressure(ByVal bChecked As Boolean) As Double
If bChecked = True Then
   PenaltySubPressure = 0.5
ElseIf PenaltySubPressure = False Then
   PenaltySubPressure = 0
End If
End Function
```

C.1. Tanks Farms Storage Flammable Liquids (for storage)

```
Function PenaltyTanks(ByVal IndexCombo As Double, ByVal bChecked As Boolean)
As Double
 Select Case IndexCombo
  Case 1:
   PenaltyTanks = 0
  Case 2:
   PenaltyTanks = 0.5
  Case 3:
   PenaltyTanks = 0.5
  End Select
```

```
  If bChecked = True Then
 PenaltyTanks = 0
 End If
End Function
```

Description to C.1
```
Function DetailTanks(ByVal dtype As Double)
If dtype = 2 Then
   DetailTanks = "Air can be breathed during pump-out or sudden cooling of the tank."
ElseIf dtype = 3 Then
   DetailTanks = "OPRS = Operating pressure-vacuum relief system"
Else
   DetailTanks = ""
End If
End Function
```

C.2. Process Upset of Purge Failure (for process equipment)
```
Function PenaltyUpset(ByVal Upset As Double) As Double
 Select Case Upset
  Case 1:
   PenaltyUpset = 0
  Case 2:
   PenaltyUpset = 0.3
  Case 3:
   PenaltyUpset = 0.3
  Case 4:
   PenaltyUpset = 0.3
  Case 5:
   PenaltyUpset = 0.3
  End Select
 End Function
```

Description to C.2

Function DetailUpset(ByVal dtype As Double)

If dtype = 2 Then

  DetailUpset = "PE is Process Equipment and PST is Process Storage Tanks"

ElseIf dtype = 3 Then

  DetailUpset = "PU is Process Units"

Else

  DetailUpset = ""

End If

End Function

C.3. Always in Flammable Range

Function PenaltyAlways(ByVal bChecked As String) As Double

If bChecked = True Then

 PenaltyAlways = 0

Else

 PenaltyAlways = 0.8

 End If

End Function

D. Dust Explosion

Function PenaltyDust(ByVal dtype As String) As Double

 If dtype = 1 Then

  PenaltyDust = 0

 ElseIf dtype = 2 Then

  PenaltyDust = 0.25

 ElseIf dtype = 3 Then

  PenaltyDust = 0.5

 ElseIf dtype = 4 Then

  PenaltyDust = 0.75

```
  ElseIf dtype = 5 Then
    PenaltyDust = 1.25
  ElseIf dtype = 6 Then
    PenaltyDust = 2
  End If
End Function
```

E. Pressure

```
Function PenaltyPressure(ByVal dtype As Double) As Double
  If (0 < dtype And dtype < 0.66) Then
    PenaltyPressure = 0
  ElseIf (0.66 <= dtype And dtype < 1000) Then
    PenaltyPressure = 0.16109 + 1.61503 * (dtype / 1000) - 1.42879 * (dtype / 1000) ^ 2
+ 0.5172 * (dtype / 1000) ^ 3
  ElseIf (1000 <= dtype And dtype <= 1500) Then
    PenaltyPressure = 0.86
  ElseIf (1500 <= dtype And dtype <= 2000) Then
    PenaltyPressure = 0.92
  ElseIf (2000 < dtype And dtype <= 2500) Then
    PenaltyPressure = 0.96
  ElseIf (2500 < dtype And dtype <= 3000) Then
    PenaltyPressure = 0.98
  ElseIf (3000 < dtype And dtype <= 10000) Then
    PenaltyPressure = 1.25
  ElseIf (dtype > 10000) Then
    PenaltyPressure = 1.5
  End If
  End Function
```

Penalty to Pressure adjustment

```
Function adjusment(ByVal dtype As String) As Double
  If dtype = 1 Then
    adjusment = 0.7
  ElseIf dtype = 2 Then
    adjusment = 1.2
  ElseIf dtype = 3 Then
    adjusment = 1.2
  ElseIf dtype = 4 Then
    adjusment = 1.3
  ElseIf dtype = 5 Then
    adjusment = 1#
  End If
End Function
```

F. Penalty to Low Temperature

```
Function PenaltyLow(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyLow = 0.3
  ElseIf dtype = 2 Then
    PenaltyLow = 0.2
  ElseIf dtype = 3 Then
    PenaltyLow = 0
  ElseIf dtype = 4 Then
    PenaltyLow = 0
  End If
End Function
```

G.1 Penalty to Liquids or Gases in Process

```
Function PenG1(ByVal dtype As Double, ByVal W1 As Double, ByVal W2 As Double,
HC1 As Double, HC2 As Double) As Double
```

'Liquids or Gases in Storage (Outside The Process Area)

W = W1

HC = HC1

If W2 > W Then

　W = W2

　HC = HC2

End If

HC = HC / 10 ^ 6

P = W * HC

　If (dtype <= 5) And (dtype >= 1) Then

　　PenG1 = 10 ^ (0.17179 + 0.42988 * Application.Log(P) - 0.37244 * (Application.Log(P)) ^ 2 + 0.177121 * (Application.Log(P)) ^ 3 - 0.029984 * (Application.Log(P)) ^ 4)

　ElseIf dtype = 6 Then

　　PenG1 = 0

　End If

End Function

G.2. Penalty to Liquid or Gases in Storage (Outside the Process Area)

Function PenaltyG2(ByVal dtype As Double, ByVal P As Double) As Double

'Liquids or Gases in Storage (Outside The Process Area)

　If dtype = 1 Then

　　PenaltyG2 = 10 ^ (-0.289069 + 0.472171 * Application.Log(P) - 0.074585 * (Application.Log(P)) ^ 2 - 0.018641 * (Application.Log(P) ^ 3))

　ElseIf dtype = 2 Then

　　PenaltyG2 = 10 ^ (-0.403115 + 0.378703 * Application.Log(P) - 0.046402 * (Application.Log(P)) ^ 2 - 0.015379 * (Application.Log(P) ^ 3))

　ElseIf dtype = 3 Then

　　PenaltyG2 = 10 ^ (-0.558394 + 0.363321 * Application.Log(P) - 0.057296 * (Application.Log(P)) ^ 2 - 0.010759 * (Application.Log(P) ^ 3))

　ElseIf dtype = 4 Then

　　PenaltyG2 = 0

```
  End If
End Function


```

G.3. Penalty to Combustible Solids in Storage/Dust in Process

```
Function PenaltyG3(ByVal dtype As Double, ByVal P As Double) As Double
'Liquids or Gases in Storage (Outside The Process Area)
  On Error GoTo err
  PenaltyG3 = 0
  If dtype = 1 Then
    PenaltyG3 = 10 ^ (0.280423 + 0.464559 * Application.Log(P) - 0.28291 * (Application.Log(P)) ^ 2 + 0.066218 * (Application.Log(P) ^ 3))
  ElseIf dtype = 2 Then
    PenaltyG3 = 10 ^ (-0.358311 + 0.453326 * Application.Log(P) - 0.141022 * (Application.Log(P)) ^ 2 + 0.02276 * (Application.Log(P) ^ 3))
  ElseIf dtype = 3 Then
    PenaltyG3 = 10 ^ (0.280423 + 0.464559 * Application.Log(6 * P) - 0.28291 * (Application.Log(6 * P)) ^ 2 + 0.066218 * (Application.Log(6 * P) ^ 3))
  ElseIf dtype = 4 Then
    PenaltyG3 = 0
  End If
err:
End Function


```

H. Penalty to Corrosion and Erosion

```
Function PenaltyCorrosion(ByVal dtype As String) As Variant
  If dtype = 1 Then
    PenaltyCorrosion = 0.1
  ElseIf dtype = 2 Then
    PenaltyCorrosion = 0.2
  ElseIf dtype = 3 Then
    PenaltyCorrosion = 0.5
  ElseIf dtype = 4 Then
```

```
  PenaltyCorrosion = 0.75
ElseIf dtype = 5 Then
  PenaltyCorrosion = 0.2
ElseIf dtype = 6 Then
  PenaltyCorrosion = 0
End If
End Function
```

I. Penalty to Leakage-Joints and Packing

```
Function PenaltyLeakage(ByVal dtype As String) As Variant
  If dtype = 1 Then
    PenaltyLeakage = 0.1
  ElseIf dtype = 2 Then
    PenaltyLeakage = 0.3
  ElseIf dtype = 3 Then
    PenaltyLeakage = 0.3
  ElseIf dtype = 4 Then
    PenaltyLeakage = 0.4
  ElseIf dtype = 5 Then
    PenaltyLeakage = 1.5
  ElseIf dtype = 6 Then
```

J. Penalty to the Use of Fired Equipment

```
Function PenaltyFired(ByVal dtype As Double, ByVal distance As Double, ByVal
Checked As Boolean) As Double
  If (distance > 210) Then
    PenaltyFired = 0.1
  ElseIf bChecked = True Then
    PenaltyFired = 0.5 * PenaltyFired
  ElseIf dtype = 1 Then
```

PenaltyFired = 10 ^ (-3.3243 * (distance / 210) + 3.75127 * (distance / 210) ^ 2 - 1.42523 * (distance / 210) ^ 3)

ElseIf dtype = 2 Then

PenaltyFired = 10 ^ (-3.3243 * (distance / 210) + 3.75127 * (distance / 210) ^ 2 - 1.42523 * (distance / 210) ^ 3)

ElseIf dtype = 3 Then

PenaltyFired = 10 ^ (-0.3745 * (distance / 210) - 2.70212 * (distance / 210) ^ 2 + 2.09171 * (distance / 210) ^ 3)

ElseIf dtype = 4 Then

PenaltyFired = 0

ElseIf dtype = 5 Then

PenaltyFired = 1

ElseIf dtype = 6 Then

PenaltyFired = 0

End If

End Function

Description to the Use of Fired Equipment

Function DetailFired(ByVal dtype As String, ByVal distance As Double) As String

If (0 <= dtype And dtype < 1000) Then

DetailFired = "if the fired equipment is the process unit being evaluated itself, the distance is zero"

End If

End Function

K. Penalty Hot Oil Exchange System

Function PenaltyHotOil(ByVal dtype As String) As Double

If dtype = 1 Then

PenaltyHotOil = 0

ElseIf dtype = 2 Then

PenaltyHotOil = 0

```
ElseIf dtype = 3 Then
  PenaltyHotOil = 0
    ElseIf dtype = 4 Then
  PenaltyHotOil = 0.15
ElseIf dtype = 5 Then
  PenaltyHotOil = 0.3
    ElseIf dtype = 6 Then
  PenaltyHotOil = 0.5
ElseIf dtype = 7 Then
  PenaltyHotOil = 0.75
    ElseIf dtype = 8 Then
  PenaltyHotOil = 0.25
ElseIf dtype = 9 Then
  PenaltyHotOil = 0.45
    ElseIf dtype = 10 Then
  PenaltyHotOil = 0.75
ElseIf dtype = 11 Then
  PenaltyHotOil = 1.05
  End If
End Function
```

L. Penalty to Rotating Equipment

```
Function PenaltyRotating(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyRotating = 0.5
  ElseIf dtype = 2 Then
    PenaltyRotating = 0.5
  ElseIf dtype = 3 Then
    PenaltyRotating = 0.5
  ElseIf dtype = 4 Then
    PenaltyRotating = 0.5
```

ElseIf dtype = 5 Then

   PenaltyRotating = 0

    End If

End Function

Description to Rotating Equipment

Function Detailrotating(ByVal dtype As String) As String

  If dtype = 3 Then

    Detailrotating = "In which failure could create a process exotherm due to lack of cooling from interupted mixing or circulation of coolant or due to interupted nad resumed mixing"

  ElseIf dtype = 4 Then

    Detailrotating = "Ex: centrifuges"

  End If

End Function

3. LOSS CONTROL CREDIT FACTOR

Process Control Credit Factor (C_1)

A. Credit to Emergency Power

Function PenaltyEmergency(ByVal dtype As String) As Double

  If dtype = 1 Then

   PenaltyEmergency = 0.98

  ElseIf dtype = 2 Then

   PenaltyEmergency = 1

  ElseIf dtype = 3 Then

   PenaltyEmergency = 1

  End If

End Function

Description to Emergency Power

Function DetailEmergency(ByVal dtype As String) As String

```
If dtype = 1 Then

    DetailEmergency = "For provision of emergency power for essential services
(instrument air control instrumentation, agitators, pumps, etc) with automatic changover
from normal to emergency. It is needed to prevent or control a possible fire/explosion
incident"

ElseIf dtype = 2 Then

    DetailEmergency = ""

End If

End Function
```

B. Credit to Cooling System

```
Function PenaltyCooling(ByVal dtype As String) As Double

  If dtype = 1 Then

    PenaltyCooling = 0.99

  ElseIf dtype = 2 Then

    PenaltyCooling = 0.97

      ElseIf dtype = 3 Then

    PenaltyCooling = 1

  End If

End Function
```

C. Credit to Explosion Control

```
Function PenaltyExplosion(ByVal dtype As String) As Double

  If dtype = 1 Then

    PenaltyExplosion = 0.84

  ElseIf dtype = 2 Then

    PenaltyExplosion = 0.98

      ElseIf dtype = 3 Then

    PenaltyExplosion = 1

  End If

End Function
```

Description to Explosion Control

```
Function DetailExplosion(ByVal dtype As String) As String
  If dtype = 1 Then
    DetailExplosion = "ESS is Explosion Suppression System"
  ElseIf dtype = 2 Then
    DetailExplosion = "ORS is Overpressure Relief System"
  End If
End Function

Function PenaltyShutdown(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyShutdown = 0.98
  ElseIf dtype = 2 Then
    PenaltyShutdown = 0.99
  ElseIf dtype = 3 Then
    PenaltyShutdown = 0.96
      ElseIf dtype = 4 Then
    PenaltyShutdown = 1
  End If
End Function
```

D. Credit to Emergency Shutdown

```
Function DetailShutdown(ByVal dtype As String) As String
  If dtype = 2 Then
    DetailShutdown = "CRE is Critical Rotating Equipment such as compressors, turbines, fans, etc, that are provided with vibration detection equipment"
  ElseIf dtype = 3 Then
    DetailShutdown = "CRE is Critical Rotating Equipment such as compressors, turbines, fans, etc, that are provided with vibration detection equipment"
  End If
End Function
```

E. Credit to Computer Control

```
Function PenaltyComputer(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyComputer = 0.99
  ElseIf dtype = 2 Then
    PenaltyComputer = 0.99
  ElseIf dtype = 3 Then
    PenaltyComputer = 0.97
  ElseIf dtype = 4 Then
    PenaltyComputer = 0.93
  ElseIf dtype = 5 Then
    PenaltyComputer = 0.93
  ElseIf dtype = 6 Then
    PenaltyComputer = 0.93
     ElseIf dtype = 7 Then
    PenaltyComputer = 1
    End If
End Function
```

F. Credit to Inert Gas

```
Function PenaltyInert(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyInert = 0.96
  ElseIf dtype = 2 Then
    PenaltyInert = 0.94
  ElseIf dtype = 3 Then
    PenaltyInert = 1
     ElseIf dtype = 4 Then
    PenaltyInert = 1
  End If
End Function
```

<u>Description to Inert Gas</u>

```
Function DetailInert(ByVal dtype As String) As String
  If dtype = 2 Then
    DetailInert = "IGS is Inert Gas System"
  ElseIf dtype = 3 Then
    DetailInert = "IGS is Inert Gas System"
  End If
End Function
```

<u>Credit to Operation Instruction/Procedure - Credit</u>

```
Function PenaltyOp1(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp1 = 0.5
  Else
    PenaltyOp1 = 0
  End If
End Function
```

```
Function PenaltyOp2(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp2 = 0.5
  Else
    PenaltyOp2 = 0
  End If
End Function
```

```
Function PenaltyOp3(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp3 = 0.5
```

```
  Else
    PenaltyOp3 = 0
  End If
End Function


Function PenaltyOp4(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp4 = 0.5
  Else
    PenaltyOp4 = 0
  End If
End Function


Function PenaltyOp5(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp5 = 0.5
  Else
    PenaltyOp5 = 0
  End If
End Function


Function PenaltyOp6(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp6 = 1
  Else
    PenaltyOp6 = 0
  End If
End Function


Function PenaltyOp7(ByVal dtype As String) As Double
  If dtype = True Then
```

```
    PenaltyOp7 = 1
  Else
    PenaltyOp7 = 0
  End If
End Function


Function PenaltyOp8(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp8 = 1
  Else
    PenaltyOp8 = 0
  End If
End Function


Function PenaltyOp9(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp9 = 1.5
  Else
    PenaltyOp9 = 0
  End If
End Function


Function PenaltyOp10(ByVal dtype As String) As Double
  If dtype = True Then
    PenaltyOp10 = 1.5
  Else
    PenaltyOp10 = 0
  End If
End Function


Function PenaltyOp11(ByVal dtype As String) As Double
```

If dtype = True Then

   PenaltyOp11 = 2

 Else

   PenaltyOp11 = 0

 End If

End Function

Function PenaltyOp12(ByVal dtype As String) As Double

 If dtype = True Then

   PenaltyOp12 = 3

 Else

   PenaltyOp12 = 0

 End If

End Function

Point for Operation Instruction/Procedure - Points

Function Point(ByVal dtype As String, ByVal IndexCombo As Byte, ByVal bChecked As Boolean) As Double

 If dtype = True Then

  a = 0.5

  b = 0.5

  c = 0.5

  d = 0.5

 Else

  Pointa = 0

 End If

End Function

H. Credit to Reactive Chemical Review

Function PenaltyReactive(ByVal dtype As String) As Double

 If dtype = 1 Then

    PenaltyReactive = 0.91
  ElseIf dtype = 2 Then
    PenaltyReactive = 0.98
  ElseIf dtype = 3 Then
    PenaltyReactive = 1
  End If
End Function

I. Credit to Other Process Hazards Analysis
Function PenaltyAnalysis(ByVal dtype As String) As Double
  If dtype = 1 Then
    PenaltyAnalysis = 0.91
  ElseIf dtype = 2 Then
    PenaltyAnalysis = 0.93
  ElseIf dtype = 3 Then
    PenaltyAnalysis = 0.93
  ElseIf dtype = 4 Then
    PenaltyAnalysis = 0.94
  ElseIf dtype = 5 Then
    PenaltyAnalysis = 0.94
  ElseIf dtype = 6 Then
    PenaltyAnalysis = 0.96
  ElseIf dtype = 7 Then
    PenaltyAnalysis = 0.96
  ElseIf dtype = 8 Then
    PenaltyAnalysis = 0.98
  ElseIf dtype = 9 Then
    PenaltyAnalysis = 0.98
  End If
End Function

4. PROCESS UNIT RISK ANALYSIS

5. Determination of Damage Factor

Function DamageFactor(ByVal dtype As Double, ByVal P As Double) As Double

'P = process unit hazards factor, dtype = material factor

  If P > 8 Then

    P = 8

  ElseIf P < 8 And P = 8 Then

    P = P

  End If

  If dtype = 1 Then

    DamageFactor = 0.003907 + 0.002957 * P + 0.004031 * P ^ 2 - 0.00029 * P ^ 3

  ElseIf dtype = 4 Then

    DamageFactor = 0.025817 + 0.019071 * P - 0.00081 * P ^ 2 - 0.000108 * P ^ 3

  ElseIf dtype = 10 Then

    DamageFactor = 0.098582 + 0.017596 * P + 0.000809 * P ^ 2 - 0.000013 * P ^ 3

  ElseIf dtype = 14 Then

    DamageFactor = 0.20592 + 0.018938 * P + 0.007628 * P ^ 2 - 0.00057 * P ^ 3

  ElseIf dtype = 16 Then

    DamageFactor = 0.256741 + 0.019886 * P + 0.011055 * P ^ 2 - 0.00088 * P ^ 3

  ElseIf dtype = 21 Then

    DamageFactor = 0.340314 + 0.076531 * P + 0.003912 * P ^ 2 - 0.00073 * P ^ 3

  ElseIf dtype = 24 Then

    DamageFactor = 0.395755 + 0.096443 * P - 0.001351 * P ^ 2 - 0.00038 * P ^ 3

  ElseIf dtype = 29 Then

    DamageFactor = 0.484766 + 0.094288 * P - 0.00216 * P ^ 2 - 0.00031 * P ^ 3

  ElseIf dtype = 40 Then

    DamageFactor = 0.554175 + 0.080772 * P + 0.000332 * P ^ 2 - 0.00044 * P ^ 3

  End If

End Function

9. Calculation of MPDO

Function MPDO(ByVal dtype As Byte, ByVal MPPD As Double, ByVal factor As Double) As Double

  If dtype = 1 Then

    MPDO = 10 ^ (1.550233 + 0.598416 * Application.Log(MPPD / 10 ^ 6))

  ElseIf dtype = 2 Then

    MPDO = 10 ^ (1.325132 + 0.592471 * Application.Log(MPPD / 10 ^ 6))

  ElseIf dtype = 3 Then

    MPDO = 10 ^ (1.045515 + 0.610426 * Application.Log(MPPD / 10 ^ 6))

  End If

  MPDO = factor * MPDO

End Function

Material Isolation Credit Factor (C_2)

A. Penalty to Remote Control Valves

Function PenaltyControl(ByVal dtype As String) As Double

  If dtype = 1 Then

    PenaltyControl = 1

  ElseIf dtype = 2 Then

    PenaltyControl = 0.98

  ElseIf dtype = 3 Then

    PenaltyControl = 0.96

  End If

End Function

Description to Remote Control Valves

Function DetailValves(ByVal dtype As Double) As String

```
If dtype = 1 Then

  DetailValves = ""

ElseIf dtype = 2 Then

  DetailValves = "ROIV = Remotely Operated Isolation Valves available to such
storage tanks, process vessles or major sections of transfer lines used in an emergency
use"

ElseIf dtype = 3 Then

  DetailValves = "ROIV = Remotely Operated Isolation Valves available to such
storage tanks, process vessles or major sections of transfer lines used in an emergency
use"

  End If

End Function
```

B. Penalty to Dump/Blowdown

```
Function PenaltyDump(ByVal dtype As String) As Double

  If dtype = 1 Then

    PenaltyDump = 1

  ElseIf dtype = 2 Then

    PenaltyDump = 0.98

  ElseIf dtype = 3 Then

    PenaltyDump = 0.96

  ElseIf dtype = 4 Then

    PenaltyDump = 0.96

  ElseIf dtype = 5 Then

    PenaltyDump = 0.98

  End If

End Function
```

Description to Dump/Blowdown

```
Function DetailDump(ByVal dtype As Double) As String

  If dtype = 1 Then

    DetailDump = ""
```

ElseIf dtype = 2 Then

DetailDump = "Emergency dump tank can be used directly to receive the contents of the process unit safely with adequate quenching and venting"

ElseIf dtype = 3 Then

DetailDump = "Emergency dump tank can be used directly to receive the contents of the process unit safely with adequate quenching and venting"

ElseIf dtype = 4 Then

DetailDump = "For Emergency venting, gas/vapor material is piped to a flare system or to a close vent receiver"

ElseIf dtype = 5 Then

DetailDump = "For normal venting that reduces the exposure of surrounding equipment to released gases or liquids. Ex: Blowdown from polystyrene reactor to a tank or receiver"

End If

End Function

Description to Drainage

Function DetailDrainage(ByVal dtype As Double) As String

If dtype = 1 Then

DetailDrainage = ""

ElseIf dtype = 2 Then

DetailDrainage = "Provide slope of at least 2% (1% on a hards surface) leading to drainage trench of adquate size. Assume 100% the content of the largest tank + 10 % of the next largest tank could be released plus 1 hr of deluge/sprinkler fire water"

ElseIf dtype = 3 Then

DetailDrainage = "Drainage could drain the contents away from under or near tanks and equipment"

ElseIf dtype = 4 Then

DetailDrainage = ""

ElseIf dtype = 5 Then

DetailDrainage = ""

ElseIf dtype = 6 Then

DetailDrainage = "The slope is doubtful or if the impounding basin < 50 ft (15 m) away"

ElseIf dtype = 7 Then

DetailDrainage = "Diking design directs spill to an impounding basin min 50 ft (15 m) away and capable of receiving 100% the content of the largest tank + 10 % of the next largest tank could be released plus 1 hr of deluge/sprinkler fire water"

End If

End Function

D. Penalty to Interlock

Function PenaltyInterlock(ByVal dtype As String) As Double

If dtype = 1 Then

PenaltyInterlock = 1

ElseIf dtype = 2 Then

PenaltyInterlock = 0.98

ElseIf dtype = 3 Then

PenaltyInterlock = 0.98

End If

End Function

Fire Protection Credit Factor (C_3)

A. Credit to Leak Detection

Function PenaltyLeak(ByVal dtype As Variant) As Variant

If dtype = 1 Then

PenaltyLeak = 1

ElseIf dtype = 2 Then

PenaltyLeak = 0.98

ElseIf dtype = 3 Then

PenaltyLeak = 0.94

End If

End Function

B. Credit to Structure Steel

```
Function PenaltySteel(ByVal dtype As Variant) As Variant
  If dtype = 1 Then
    PenaltySteel = 1
  ElseIf dtype = 2 Then
    PenaltySteel = 0.98
  ElseIf dtype = 3 Then
    PenaltySteel = 0.97
  ElseIf dtype = 4 Then
    PenaltySteel = 0.95
  ElseIf dtype = 5 Then
    PenaltySteel = 0.98
  ElseIf dtype = 6 Then
    PenaltySteel = 0.98
  End If
End Function
```

C. Credit to Fire Water Supply

```
Function PenaltyWater(ByVal dtype As Variant) As Variant
  If dtype = 1 Then
    PenaltyWater = 1
  ElseIf dtype = 2 Then
    PenaltyWater = 0.94
  ElseIf dtype = 3 Then
    PenaltyWater = 0.97
  ElseIf dtype = 4 Then
    PenaltyWater = 0.97
  End If
End Function
```

Description to Fire Water Supply

Function DetailWater(ByVal dtype As Double) As String

  If dtype = 2 Then

    DetailWater = "Applicable to fire water supply provided by alternative power source, independent of normal electric service and deliver maximum demand"

  ElseIf dtype = 3 Then

    DetailWater = "Applicable to fire water supply provided by alternative power source, independent of normal electric service and deliver maximum demand"

  ElseIf dtype = 4 Then

    DetailWater = "Applicable to fire water supply provided by alternative power source, independent of normal electric service and deliver maximum demand"

  End If

End Function

D. Credit to Special Systems

Function PenaltySpecial(ByVal dtype As Variant) As Variant

  If dtype = 1 Then

    PenaltySpecial = 1

  ElseIf dtype = 2 Then

    PenaltySpecial = 0.91

  End If

End Function

Description to Special System

Function DetailSpecial(ByVal dtype As Double) As String

  If dtype = 1 Then

    DetailSpecial = ""

  ElseIf dtype = 2 Then

    DetailSpecial = "Special system include CO2, Halon, smoke, and flame detectors and blast walls or cubicle, double wall for outer tank and buried tank (discouraged)"

  End If

End Function

E. Credit to Sprinkler System - Design

Function PenaltyDesign(ByVal dtype As Variant) As Variant

  If dtype = 1 Then

    PenaltyDesign = 1

  ElseIf dtype = 2 Then

    PenaltyDesign = 0.87

  ElseIf dtype = 3 Then

    PenaltyDesign = 0.87

  ElseIf dtype = 4 Then

    PenaltyDesign = 0.81

  ElseIf dtype = 5 Then

    PenaltyDesign = 0.84

  ElseIf dtype = 6 Then

    PenaltyDesign = 0.74

  ElseIf dtype = 7 Then

    PenaltyDesign = 0.81

  End If

End Function

E. Penalty to Sprinkler System - Area

Function PenaltyArea(ByVal Credit As Double, ByVal Area As Double) As Double

Select Case Credit

  Case 1:

    PenaltyArea = 1

  Case 2:

    PenaltyArea = 0.87

  Case 3:

    PenaltyArea = 0.87

  Case 4:

```
    PenaltyArea = 0.81
  Case 5:
    PenaltyArea = 0.84
  Case 6:
    PenaltyArea = 0.74
  Case 7:
    PenaltyArea = 0.81
End Select


 If Area = 2 Then
   PenaltyArea = PenaltyArea * 1.06
 ElseIf Area = 3 Then
   PenaltyArea = PenaltyArea * 1.09
 ElseIf Area = 4 Then
   PenaltyArea = PenaltyArea * 1.12
 End If
End Function
```

F. Penalty to Water Curtain

```
Function PenaltyCurtain(ByVal dtype As Variant) As Variant
  If dtype = 1 Then
    PenaltyCurtain = 1
  ElseIf dtype = 2 Then
    PenaltyCurtain = 0.98
  ElseIf dtype = 3 Then
    PenaltyCurtain = 0.97
   End If
End Function
```

Description to Water Curtain

```
Function DetailCurtain(ByVal dtype As Double) As String
```

```
   If dtype = 2 Then

      DetailCurtain = "Appicable to Automatic water spray between source of ignition and a
potential vapor release area and located at least 75 ft (23 m) from the vapor release
point"""

   ElseIf dtype = 3 Then

      DetailCurtain = "Appicable to Automatic water spray between source of ignition and a
potential vapor release area and located at least 75 ft (23 m) from the vapor release
point"""

   End If

End Function
```

G. Penalty to Foam

```
Function PenaltyFoam(ByVal dtype As Variant) As Variant

   If dtype = 1 Then

     PenaltyFoam = 1

   ElseIf dtype = 2 Then

     PenaltyFoam = 0.94

   ElseIf dtype = 3 Then

     PenaltyFoam = 0.92

   ElseIf dtype = 4 Then

     PenaltyFoam = 0.97

   ElseIf dtype = 5 Then

     PenaltyFoam = 0.94

   ElseIf dtype = 6 Then

     PenaltyFoam = 0.95

   ElseIf dtype = 7 Then

     PenaltyFoam = 0.97

   ElseIf dtype = 7 Then

     PenaltyFoam = 0.94

   End If

End Function
```

Description to Foam

Function DetailFoam(ByVal dtype As Double) As String

  If dtype = 3 Then

    DetailFoam = "Automatically means the foam valve is automatically actuated when fire is detected"

  ElseIf dtype = 5 Then

    DetailFoam = "Automatic means fire detection systems are used to actuating the foam system"

  End If

End Function

H. Penalty to Hand Extinguisher/Monitors

Function PenaltyHand(ByVal dtype As Variant) As Variant

  If dtype = 1 Then

   PenaltyHand = 1

  ElseIf dtype = 2 Then

   PenaltyHand = 0.98

  ElseIf dtype = 3 Then

   PenaltyHand = 1

  ElseIf dtype = 4 Then

   PenaltyHand = 1

  ElseIf dtype = 5 Then

   PenaltyHand = 0.97

  ElseIf dtype = 6 Then

   PenaltyHand = 0.95

  ElseIf dtype = 7 Then

   PenaltyHand = 0.93

  End If

End Function

I. Penalty to Cable Protection

```
Function PenaltyCable(ByVal dtype As Variant) As Variant
  If dtype = 1 Then
    PenaltyCable = 1
  ElseIf dtype = 2 Then
    PenaltyCable = 0.98
  ElseIf dtype = 3 Then
    PenaltyCable = 0.98
  ElseIf dtype = 4 Then
    PenaltyCable = 0.94
   End If
End Function
```

Description to Cable Protection

```
Function DetailCable(ByVal dtype As Double) As String
  If dtype = 2 Then
    DetailCable = "Completed with water spray directed onto the top side"
  ElseIf dtype = 4 Then
    DetailCable = "Applicable for both flooded or dry"
   End If
End Function
```

MATERIAL FACTOR DETERMINATION FOR UNLISTED SUBSTANCES

Material Factor for Liquids and Gases Flammability or Combustibility and Volatile Solids

```
Option Base 1

Function Reactivity(ByVal NR As Integer, ByVal NF As Integer)

Dim NF0 As Variant, NF1 As Variant, NF2 As Variant, NF3 As Variant, NF4 As Variant
```

NF0 = Array(1, 14, 24, 29, 40)

NF1 = NF0

NF1(1) = 4

NF2 = NF0

NF2(1) = 10

NF3 = NF0

NF3(1) = 16: NF3(2) = 16

NF4 = NF0

NF4(1) = 21: NF3(2) = 21

Select Case NF

  Case 0: Reactivity = NF0(NR + 1)

  Case 1: Reactivity = NF1(NR + 1)

  Case 2: Reactivity = NF2(NR + 1)

  Case 3: Reactivity = NF3(NR + 1)

  Case 4: Reactivity = NF4(NR + 1)

End Select

End Function

NF determination for Liquids and Gases Flammability or Combustibility and Volatile Solids

Function Nflam(ByVal InputCombo As String) As Double

  Select Case InputCombo

  Case 1:

    Nflam = 0

  Case 2:

    Nflam = 0

```
    Case 3:
      Nflam = 1
    Case 4:
      Nflam = 2
    Case 5:
      Nflam = 3
    Case 6:
      Nflam = 3
    Case 7:
      Nflam = 4


  End Select
End Function
```

Material Factor for Combustible Dust or Mists

```
Function Dust(ByVal NR As Integer, ByVal NF As Integer)

Dim NF0 As Variant, NF1 As Variant, NF2 As Variant, NF3 As Variant, NF4 As
Variant

NF0 = Array(16, 16, 24, 29, 40)


NF1 = NF0


NF2 = NF0
NF2(1) = 21: NF2(2) = 21


NF3 = NF0
NF3(1) = 24: NF3(2) = 24


Select Case NF
  Case 0: Dust = NF0(NR + 1)
```

```
   Case 1: Dust = NF1(NR + 1)
   Case 2: Dust = NF2(NR + 1)
   Case 3: Dust = NF3(NR + 1)
   Case 4: Dust = NF4(NR + 1)
End Select
End Function
```

Dust Class Determination

```
Function Stvalue(ByVal InputCombo As String, ByVal user As Double) As Double
  Select Case InputCombo
   Case 1:
    Stvalue = 1
   Case 2:
    Stvalue = 2
   Case 3:
    Stvalue = 3
   Case 4:
    Stvalue = user
  End Select
End Function
```

Material Factor for Combustible Solids

```
Function Solids(ByVal NR As Integer, ByVal NF As Integer)
Dim NF0 As Variant, NF1 As Variant, NF2 As Variant, NF3 As Variant, NF4 As Variant

NF0 = Array(4, 14, 24, 29, 40)


NF1 = NF0


NF2 = NF0
NF2(1) = 10
```

NF3 = NF0

NF3(1) = 10: NF3(2) = 14

NF4 = NF0

NF4(1) = 16: NF3(2) = 16

Select Case NF

  Case 0: Solids = NF0(NR + 1)

  Case 1: Solids = NF1(NR + 1)

  Case 2: Solids = NF2(NR + 1)

  Case 3: Solids = NF3(NR + 1)

  Case 4: Solids = NF4(NR + 1)

End Select

End Function

N_F for Combustible Solids

Function SolidsVal(ByVal InputCombo As String, ByVal user As Double) As Double

  Select Case InputCombo

  Case 1:

   SolidsVal = 1

  Case 2:

   SolidsVal = 2

  Case 3:

   SolidsVal = 3

  Case 4:

   SolidsVal = user

  Case 5:

   SolidsVal = 1

  Case 6:

   SolidsVal = 1

```
Case 7:
  SolidsVal = 1
Case 8:
  SolidsVal = 1
Case 9:
  SolidsVal = 2
Case 10:
  SolidsVal = 2
Case 11:
  SolidsVal = 2
Case 12:
  SolidsVal = 1
Case 13:
  SolidsVal = 3
Case 14:
  SolidsVal = 3
Case 15:
  SolidsVal = 3
Case 16:
  SolidsVal = 3
End Select
End Function



  PenaltyLeakage = 0
 End If
End Function
```

NR Determination

```
Function UnlistedSubs(ByVal IndexCombo As String, ByVal bChecked As Boolean) As
Double
```

```
Select Case IndexCombo
 Case 1:
   UnlistedSubs = 0
 Case 2:
   UnlistedSubs = 0
 Case 3:
   UnlistedSubs = 0
 Case 4:
   UnlistedSubs = 1
 Case 5:
   UnlistedSubs = 1
 Case 6:
   UnlistedSubs = 2
 Case 7:
   UnlistedSubs = 2
 Case 8:
   UnlistedSubs = 2
 Case 9:
   UnlistedSubs = 3
 Case 10:
   UnlistedSubs = 3
 Case 11:
   UnlistedSubs = 3
 Case 12:
   UnlistedSubs = 4
 Case 13:
   UnlistedSubs = 4
 Case 14:
   UnlistedSubs = 4

End Select
```

```
  If UnlistedSubs = 4 Then
    UnlistedSubs = 4
  ElseIf bChecked = True Then
    UnlistedSubs = UnlistedSubs + 1
  End If
End Function
```

F&EI Severity Determination on the F&EI Table

```
Function FEI(ByVal dtype As Double) As String
  If (1 < dtype And dtype <= 60) Then
    FEI = "Light"
  ElseIf (61 <= dtype And dtype <= 96) Then
    FEI = "Moderate"
  ElseIf (96 < dtype And dtype <= 127) Then
    FEI = "Intermediate"
  ElseIf (127 < dtype And dtype <= 158) Then
    FEI = "HEAVY"
  ElseIf (dtype > 158) Then
    FEI = "SEVERE"
  End If
End Function
```

STORING KNOWN DATA AS DATABASES

```
Sub StoreIntoBlankRow()
Dim i As Long
Dim BlankRow  As Long

Dim NewData As Range
Set NewData = Range("NewData")
```

```
With Sheets("Chemicals")
For i = 12 To 64000
   If Len(.Range("A" & i)) = 0 And Len(.Range("B" & i)) = 0 Then
      BlankRow = i
      Exit For
   End If
Next


For i = 2 To NewData.Rows.Count
   .Cells(BlankRow, i - 1) = NewData.Cells(i, 1)
Next
End With


Call AdjustInputRange(BlankRow)
End Sub
```

THE AMOUNT OF MATERIAL (LB) AND PRESSURE (PSIG) VERSUS F&EI VALUE

```
Sub SensMaterialWeight()
Dim matValOr As Double
matValOr = Range("materialval")
With Sheets("F&EI Table")
For i = 9 To 20000
  If .Range("G" & i) = 0 Or .Range("G" & i) = "" Then Exit For
     Range("materialval") = .Range("G" & i)
     .Range("H" & i).Select
     .Range("H" & i) = Range("ControlVar")
Next
Range("ControlVar").Select
```

```
Range("materialval") = matValOr
End With



matValOr = Range("pressval")
With Sheets("F&EI Table")
For i = 9 To 20000
  If .Range("I" & i) = 0 Or .Range("I" & i) = "" Then Exit For
    Range("pressval") = .Range("I" & i)
    .Range("J" & i).Select
    .Range("J" & i) = Range("ControlVar")
Next
Range("ControlVar").Select
Range("pressval") = matValOr
End With



matValOr = Range("tempval")
With Sheets("F&EI Table")
For i = 9 To 20000
  If .Range("K" & i) = 0 Or .Range("K" & i) = "" Then Exit For
    Range("tempval") = .Range("K" & i)
    .Range("L" & i).Select
    .Range("L" & i) = Range("ControlVar")
Next
Range("ControlVar").Select
Range("tempval") = matValOr
End With

End Sub
```

APPENDIX B

ALGORITHMS FOR LINGO: REACTOR-DISTILLATION COLUMN SYSTEM

1. REACTOR

```
Min=TotalCapitalInvestment;

TotalCapitalInvestment=11.68*Cp;

Cp=Cv+Cpl;
Cv=-2E-07*W^2+1.0346*W+45564;

Cpl=285.1*(Di)^0.73960*(L)^0.70684;
W=0.25326*(Di*12+tp)*(L*12+9.6*Di)*tp; !for Carbon steel, 0.284
lb/inch3;
tp=(Pd*Di*12)/(25500-1.2*Pd); !(inches);
Pd=-9E-05*Po^2+1.1751*Po+12.872;

!CONSTRAINT (economic);
tp>0;
!tp<0.25;

Di>3; ![=]ft;
Di<21; ![=]ft;
L<40; ![=]ft;
W<920000; ![=]lb;


!Volume of Reactor vs Conversion of A ----> B, Plug Flow Reactor, gas
phase, Constant temperature;

Cao*1445=P; !p[=]atm;
Po=(P*14.7)-14.7; !po[=]psig;
P>2;
P<8;
Cao*2.355*L*Di^2=Fao*(2*@LOG(1/(1-X))-X);
Volume=Cao*2.355*L*Di^2;

Fao=Fb/X; ![=] lb mol/s;
Fb=0.40;

X=0.4;

FEI1=3*10^-8*(Wr)^2+0.0012*(Wr)+88.46; !Wr[=]lb;
Wr=Fao*26400; !Wr[=]lb, Fao[=]lb/10 minute;
FEI2=0.1176*Po+109.8; !Po[=]psig;

FEI1>0;
FEI1<128;
FEI2>0;
```

```
FEI2<128;
```

2. DISTILLATION COLUMN

```
Min=TotalCost;


Vm=1080*((44-rhogt)/rhogt)^0.5; !ft/hr;
Did=((56.051*600)/(rhogt*Vm))^0.5; !Didt[=]ft;
rhogt*1445=P; !P[=]atm, ;
Pod=(P*14.7)-14.7; !po[=]psig;

P>10;
P<16;

FEI3=-1E-08*Wr3^2+ 0.0018*Wr3+101.16;
Wr3=7.33*Fao*Xf; !Wr[=]lb, Fao[=]lb for 10 minute;
FEI4=5E-05*Po^2+0.1072*Po+106.83; !Po[=]psig;

!CONSTRAINT (safety parameters);
FEI3>0;
FEI3<128;
FEI4>0;
FEI4<128;



TotalCost=6.68*DistillationCost+OperatingCost;
OperatingCost=780*V;
Distillationcost=Ct+Cpd;

Cpd=Cvd+Cpld;
Wd=0.25326*(Did*12+tpd)*(hd*12+9.6*Did)*tpd;
tpd=(Pdd*Did*12)/(25500-1.2*Pdd);
Pdd=1.1038*(Pod)+21.903; !Pdd[=] psig;
Cvd=0.9295*(Wd) + 174525;
Cpld=237.1*((Did)^0.63316)*(hd^0.8061);

Ct=N*Cbt; !Ftm=1; !Carbon steel, FTT=1, Sieve tray);
Cbt=4.1192*Did^3 - 91.738*Did^2 + 876.76*Did - 1598.2;

Fao=1440;
B>0;
Xd=0.95;

Xb=0.05;
Xf=0.2;

R=18.77;
N=95;

1440=D+B;
1440*Xf=Xd*D+Xb*B;
```

```
R*D=L;
V=(R+1)*D;
```

VITA

Jaffee Suardin was born as the 2nd child to Mr. Suardin, a chemical engineer, and Mrs. Linggardjati Suardin in Palembang, South Sumatera, Indonesia in December 21, 1977. He lived in the Fertilizer Company Residency in Palembang, Indonesia until he graduated from SMAN I High School. He was interested in chemical engineering and pursued a degree at Bandung Institute of Technology in Bandung in 1996, West Java, Indonesia.

He graduated with a B.S. degree in chemical engineering in 2002. He applied to Texas A&M University and started the Master of Science program in Fall 2003. In spring 2004, he joined the Mary Kay O'Connor Process Safety Center at Texas A&M University and began working on his research under the guidance of Dr. M. Sam Mannan. He received his M.S. degree in chemical engineering in August 2005.

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