

**INHERENT SAFETY COST INDEX (ISCI) FOR PRELIMINARY PROCESS
DESIGN**

by

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Dissertation submitted in partial fulfillment of
the requirements for the
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CERTIFICATION OF APPROVAL

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Approved by,

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CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

NUR HIDAYAH BT MANSOR

ABSTRACT

Inherent safety principles were first introduced by Trevor Kletz in 1976 after Flixborough accident. The inherent safety principles include minimization, substitution, attenuation, simplification, and limiting of. Implementing inherent safety in the design aims at selecting and designing the process to eliminate hazards, in contrary to passive control which accepts the hazards and implementing add-on systems to control them. Inherent safety is best considered in the initial stages of the design when fundamentals decisions which have a large impact on inherent safety are made. There are a few established models developed for inherent safety index but most of them only consider process safety. At present, the only index established which includes cost evaluation is Integrated Inherent Safety Index (I2SI). The costs to operate a plant which is built based on inherent safety principles is proven to be more economically by several writers. The project will require the application of inherent safety principles in the preliminary design which will consequently reduce the cost of losses as the probability of accident occurrence will be reduced.

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ABBREVIATIONS

PIIS	Prototype Index for Inherent Safety
ISI	Inherent Safety Index
NFPA	National Fire Protection Association
I2SI	Integrated Inherent Safety Index
ICI	Individual Chemical Index
IRI	Individual Reaction Index
TRI	Total Reaction Index
HCI	Hazardous Chemical Index
HRI	Hazardous Reaction Index
OCI	Overall Chemical Index
ORI	Overall Reaction Index
OSI	Overall Safety Index
WCI	Worst Chemical Index
WRI	Worst Reaction Index
TCI	Total Chemical Index
SWeHI	Safety Weighted Hazard Index
ISPI	Inherent Safety Potential Index
DI	Damage Index
PHCI	Process and Hazard Control Index
CSCI	Conventional Safety Cost Index
ISCI	Inherent Safety Cost Index
ROI	Return On Investment
FCI	Fixed Capital Investment
WC	Working Capital
TCI	Total Capital Investment

CHAPTER 1: INTRODUCTION

The inherent safety principles were introduced by Trevor Kletz after 28 people had died of Flixborough accident in 1974. He had introduced the concept through his books and papers. The interest was limited at first, but Bhopal incident which causes 3800 fatalities and approximately 11000 to be disabled had given greater impact to more serious discussion on inherent safety [1].

Process design is aimed to create an economical, safe and environmentally benign throughout the plant lifetime. A certain level of safety should be reached in each process plant due to the general society requirements, company image, and also economical reasons. Large potential losses of production and capital cause an unsafe plant to be non-profitable. The safety level of a chemical process can be achieved through inherent (internal) and external means. The inherent safety is related to removing hazards rather than to controlling them by added-on protective system, which is the principle of external safety- [2].

3.1

Major decisions which influence many aspects are decided during the process development and conceptual design phases. In most of the cases, safety aspect is considered at the very last stage of design development and often it includes passive control for hazardous conditions. For example, current control measure to control for high pressure vessel is by usage of relieve valve. Inherent safety works to remove the hazardous condition (in this example, high pressure) to less hazardous conditions (atmospheric pressure) so that there is no severe injury if explosion (which is less likely) happens.

It has been proven that, considering the lifetime costs of a process and its operation, an inherently safer approach is a cost-optimal option [3]. Lifetime costs include the fixed cost of the facility, operations costs, maintenance, and safety measures [4]. Conventional systems may be cheaper in terms of fixed and operational costs; however, considering maintenance and safety measure costs, these systems may turn out to be costlier than those based on the principles of inherent safety (which may well have higher fixed costs). There are numerous examples in the process industries for such situations [4,5]. Inherent safety can be incorporated at any stage of design and operation; however, its application at the earliest possible stages of process design yields the best results [6,7].

Intuitively, inherently safer designs offer cost savings and profit enhancement [8]. Smaller inventory means smaller vessels are required, which means less cost is spent, thus reducing the inventory cost. Meanwhile, less unit equipment and auxiliary equipment in the design simply means cost spent for capital cost is less. By avoiding hazards in the process route itself, the requirement to adopt costly hazard control measures is eliminated.

- ~~• Inventory reduction will generally reduce costs because smaller vessels cost less;~~
- ~~• Simpler plant costs less because there is less equipment and ancillaries;~~
- ~~• Avoiding hazards also avoids the costly hazard control measures.~~

3.2 These arguments apply equally to capital and operating cost. By reducing count, size and complexity of equipment, the utilities, labor, testing and maintenance costs will also reduce.

Therefore, the preliminary design phase is the best opportunity to implement inherent safety principles. In fact, the possibility of implementing inherent safety decreases as the design proceeds. Thus, inherent safety characteristics should be evaluated systematically as early as possible [9].

The problem to adopt inherent safety is Lack of detailed information complicates which were needed during safety evaluation and decision-making which are conducted at the preliminary stage. At the very early stage, much of the detailed information on which the decisions should be based is still missing, because the process is still being designed. Once the required information is already available, in which the process is completely design, conceptual changes are not welcomed as they need to go through each details all over again. This paradox makes it necessary to implement a dedicated methodology for evaluating inherent safety in conceptual design to allow early adoption of its principles.

3.3 Basic design measures are used in inherent safety approach to eliminate, prevent and reduce hazard. An inherently safe plant or activity cannot (under any circumstances) cause harm to people or environment [10]. The significant features of an inherently safe plant are the usage of harmless material, small inventories of hazardous materials which are insufficient to cause significant harm even if released, and the conditions that the hazardous materials are held which make them effectively harmless (diluted, at ambient temperature and pressure, etc.) [11].

The objective of the research is to apply inherent safety in the preliminary process design. Other objective would be to show how the application of inherent safety into the process design can be related to the cost. It is the author's hope that this study will show that the adoption of inherent safety principles in the process design will give significant impact especially for the cost.

CHAPTER 2: LITERATURE REVIEW

This chapter will discuss on inherent safety principles and its development. The integrated inherent safety index will be described in details. Later, cost benefit will be explained for future understanding.

2.1 Inherent Safety Principles

Approaches to the design of inherently safer processes and plants have been grouped into four major strategies.

Principle	Description
Minimize	<ul style="list-style-type: none">▪ Applies when the hazardous materials cannot be eliminated▪ Use smaller quantities of hazardous substances, such that if a release occur, the impact is insignificant▪ Challenges process designers to determine an optimum inventory of hazardous material that compromises neither profitability nor the safety integrity of a process▪ Reduction of quantity within process area minimizes the severity and escalation of incidents (Domino's effect)
Substitute	<ul style="list-style-type: none">▪ Can be achieved in various ways ; replace a material with a less hazardous substance, replace chemical process route with one that avoids hazardous processing conditions, replace equipment with alternative equipment to eliminate an identified hazard▪ Strives to eliminate materials with highly hazardous inherent characteristics (flammability, reactivity, toxicity)
Moderate	<ul style="list-style-type: none">▪ Can be achieved by ; use less hazardous conditions, a less hazardous form of a material, the use of less severe processing conditions▪ Other method include dilution, refrigeration, secondary

Principle	Description
	containment, and temperature/pressure reduction <ul style="list-style-type: none"> ▪ Overall objectives is to eliminate or reduce hazards
Simplify	<ul style="list-style-type: none"> ▪ Involves design facilities which eliminate unnecessary complexity and make operating errors less likely, and which are forgiving of errors which are made ▪ Simpler plants contain fewer equipment which reduces the chances of material escaping into the environment ▪ Provides less opportunity for operating errors or equipment failures to occur

Table 1 Inherent safety principles [5]

2.2 Safety Indexing Development

2.2.1 Prototype Index for Inherent Safety (PIIS)

The first index published to evaluate inherent safety in process pre-design was developed by Edwards and Lawrence in 1993. It is intended for analyzing the choice of a process route and it is reaction step oriented. The index is calculated as a sum of Chemical Score and Process Score. Chemical score consists of inventory, flammability, explosiveness and toxicity meanwhile Process Score includes temperature, pressure and yield.

2.2.2 Inherent safety index (ISI)

Heikkila developed this index in 1999 which consider a larger scope of process steps, not only the reaction route but also the separation sections. The index is based on the evaluation of 12 parameters and it consists of two main index group as in Equation (1); chemical inherent safety index, I_{CI} and process inherent safety index, I_{PI}

$$I_{ISI} = I_{CI} + I_{PI} \quad (1)$$

Chemical inherent safety index, I_{CI}	Process inherent safety index, I_{PI}
--	---

Chemical inherent safety index, I_{CI}	Process inherent safety index, I_{PI}
Subindices for reaction hazards <ul style="list-style-type: none"> - Heat of the main reaction I_{RM} - Heat of the side reactions I_{RS} - Chemical interaction I_{INT} 	Subindices for process condition <ul style="list-style-type: none"> - Inventory I_I - Process temperature I_T - Process pressure I_P
Subindices for hazardous substances <ul style="list-style-type: none"> - Flammability I_{FL} - Explosiveness I_{EX} - Toxicity I_{TOX} - Corrosiveness I_{COR} 	Subindices for process system <ul style="list-style-type: none"> - Equipment I_{EQ} - Process structure I_{ST}

Table 2 inherent safety index and its subindices

The chemical inherent safety index I_{CI} as in Equation (2) contains chemical factors affecting the inherent safety of a process. These factors consist of chemical reactivity, flammability, explosiveness, toxicity and corrosiveness of the chemical substances present in the process. Flammability, explosiveness, and toxicity are determined separately for each substance in the process. Chemical reactivity consists of the maximum values of indices for the heats of both main and side reactions, and the maximum value of chemical interaction, which describes the unintended reactions between chemical substances present in the process area studied.

$$I_{CI} = I_{RM,max} + I_{RS,max} + I_{INT,max} + (I_{FL} + I_{EX} + I_{TOX})_{max} + I_{COR,max} \quad (2)$$

The process inherent safety index I_{PI} expresses the inherent safety of the process itself. It contains the subindices of inventory, process temperature and pressure, equipment safety and safe process structure. This can be calculated using Equation (3).

$$I_{PI} = I_I + I_{T,max} + I_{P,max} + I_{EQ,max} + I_{ST,max} \quad (3)$$

The index for process structure gives an opportunity to include earlier experience on similar or analog process concepts in the evaluation. If these subindices are used, it is to be estimated by an experienced designer or by using case-based reasoning techniques on accident databases.

2.2.3 *i*-Safe index

The index was developed by Palaniappan in 2002. The index compares process routes by using sub-index values from ISI and PIIS and includes NFPA reactivity rating values for chemicals present in the reaction.

For the individual reaction steps (i.e. subprocesses) the Overall Safety Index (OSI) includes Individual Chemical Index (ICI), Individual Reaction Index (IRI) and Total Reaction Index (TRI). The indices for the whole process are: Hazardous Chemical Index (HCI), Hazardous Reaction Index (HRI), Overall Chemical Index (OCI), Overall Reaction Index (ORI), Overall Safety Index (OSI), Worst Chemical Index (WCI), Worst Reaction Index (WRI), and Total Chemical Index (TCI).

ICI is determined by the properties of the chemicals involved in the reaction, and is calculated as a summation of indices assigned for flammability (N_f), toxicity (N_t), explosiveness (N_e), and NFPA reactivity rating (N_r). In ICI, all subindex values come from ISI, except the reactivity rating, which comes from NFPA reactivity rating values for chemicals.

Individual reaction index (IRI) is calculated as a summation of subindices for temperature (R_t), pressure (R_p), yield (R_y) and heat of reaction (R_h), which is quite similar to the process score for PIIS except that the heat of reaction is added. The index values, however, are taken from ISI, except the yield, which comes from PIIS.

Total reaction index (TRI) for each reaction steps (i.e. subprocesses) is the sum of IRI and the max ICI for each step. Overall safety index (OSI) is the sum of TRIs for each reaction-step and describes the inherent safety of the whole route as in Equation (4). TRI is the sum of IRI and the max ICI for each step.

$$\text{OSI} = \text{ICI} + \text{IRI} + \text{TRI} \quad (4)$$

2.2.4 Fuzzy Logic

This index developed by Gentile is also known as “fuzzy set analysis” and possibility theory”. The index works with uncertainty and imprecision and it is an efficient tool for applications where no sharp boundaries (or problem definitions) are possible. The use in different aspect of safety and reliability analysis has been discussed in a number of papers.

2.2.5 Integrated inherent safety index (I2SI)

This index developed by Faisal & Amyotte in 2005. The index considers the life cycle of the process with economic evaluation and hazard potential identification for each option. I2SI comprises of sub-indices which for account for hazard potential, inherent safety potential, and add-on control requirements. In addition to evaluate these respective characteristics, there are also indices that measure the economic potential of the option. The application of I2SI will be discussed in the next chapter.

2.3 Economic evaluation for conventional design

Economic evaluations must be done by process engineers at several stages; before a process is initiated, at various stages in its development, and before the design of a

process and plant is attempted. The evaluation decides whether the project should be undertaken, abandoned, or continued (with further research), or taken to the pilot plant stage. If the project is decided to proceed further, an economic evaluation will pinpoint those parts of the process requiring additional study. Economic evaluation of a project is a continuous procedure [12]. As the process engineer gathers new information, a more accurate evaluation can be made follow by a re-examination of the project to determine if it should continue.

Prior to operation of an industrial plant, a large sum of fund must be available to purchase and install necessary machines and equipment required for the process. Land must be obtained, service facilities must be made available, and the plant must be erected complete with all piping, instrumentations, controls and services. Besides, funds are required to pay the expenses involved in the plant operation before sales revenue becomes available.

Even if sufficient technical information is not available to design a plant completely, economical evaluation must still be made to determine if it is economically and financially feasible. A project is economically feasible when it is more profitable than other competing projects and financially feasible when management can raise the capital for its implementation [13]. Although calculations may show that a given project could be extremely profitable, the capital requirements may strain the financial capabilities of the organization. In such cases, the project may be terminated unless partners can be found to share the risk.

The process of economic evaluation consists of;

1. Prepare a process flow diagram
2. Calculate mass and energy flows
3. Size major equipment

4. Estimate the capital cost
5. Estimate production cost
6. Forecast the product sales price
7. Estimate the return on investment (ROI)

2.3.1 Fixed Capital Investment (FCI)

Fixed Capital Investment (FCI) represents the capital necessary for the installed process equipment with all components that are needed for complete process operation [14]. Fixed capital investment does not vary with production rate and have to be paid whatever the quantity produced [15]. The examples of fixed capital investment are as follows;

- i. land
- ii. processing building
- iii. administrative and other offices
- iv. warehouses
- v. laboratories
- vi. transportation
- vii. shipping
- viii. receiving facilities
- ix. utility and waste disposal facilities
- x. shops
- xi. other permanent parts of the plant

2.3.2 Working Capital (WC)

Working capital is the costs that are dependent on the amount of product produced [15] and usually are invested in [14];

- i. raw materials and supplies carried in stock
- ii. finished products oin stock and semifinished products in the process of being manufactured
- iii. accounts receivable

- iv. cash kept on hand for monthly payment of operating expenses (salaries, wages, raw material purchases)
- v. accounts payable
- vi. taxes payable

Most of the chemical plants use an initial working capital amount of 10 to 20% of the total capital investment [14]. This percentage may increase to as much as 50% or more for companies producing seasonal demand products, as the large inventories must be maintained for appreciable periods.

The sum of fixed capital investment and working capital gives total capital investment (TCI). This is shown by Equation (5);

$$TCI = FCI + WC \quad (5)$$

The total capital requirements and the production cost of a product are required for the management to determine the financial attractiveness of a process. Operating cost and manufacturing cost have been used synonymously with production cost.

Table 3 divides the total production cost into three main categories which is direct costs, indirect costs, and general costs. Direct costs which is also known as variable costs, is proportional to the production rate. The indirect cost, composed of fixed costs and plant overhead cost, remains constant regardless of the production rate. General costs include the costs of managing the firm, marketing the product, research and development on new and old products, and financing the operation.

1) Direct Costs	
1.1)	Utilities
i.	Steam
ii.	Electricity
iii.	Fuel
iv.	Refrigeration
v.	Water
vi.	Waste treatment

<ul style="list-style-type: none"> vii. Operating supplies viii. Maintenance supplies ix. Operating labor, supervision x. Maintenance labor, supervision xi. Quality Control 	
2) Indirect Costs	
2.1) Fixed Cost <ul style="list-style-type: none"> i. Royalties ii. Depreciation iii. Property taxes iv. Insurance v. Rent 	2.2) Plant Overhead Costs <ul style="list-style-type: none"> i. Indirect labor, supervision ii. Fringe benefits iii. Medical facilities iv. Fire, Safety, Security v. Waste Treatment Facilities vi. Packaging Facilities vii. Restaurant Facilities viii. Recreation Facilities ix. Salvage Services x. Quality Control Laboratory xi. Shipping, Receiving Facilities xii. Storage Facilities xiii. Maintenance Facilities
3) General Costs	
3.1) Administrative Costs <ul style="list-style-type: none"> i. Executive ii. Clerical iii. Engineering iv. Legal v. Communications 	3.2) Marketing Costs <ul style="list-style-type: none"> i. Sales ii. Advertising iii. Product distribution iv. Technical sale service v. Financing cost vi. Research and development

Table 3 Components of total production cost

2.3.3 Direct Costs

2.3.3.1 Raw Materials

Sometimes raw material cost will dominate the production cost. Raw material prices for preliminary estimates may be obtained from the supplier. Prices of chemicals depend on the quantity purchased.

2.3.3.2 Catalysts

Loss of catalyst happens because of abrasion during use and regeneration. Some of the catalyst are eventually spent and must be replaced. Thus, the cost of catalyst must be included in the production cost.

2.3.3.3 Solvents

Solvents are used in separation process, especially in solvent extraction and gas absorption and liquid-phase reactions. The solvents are usually recovered within the process and reused, but losses occur because of leaks, incomplete recovery, and degradation.

2.3.3.4 Utilities

Utilities include steam, electricity, fuel, cooling water, process water, compressed air, refrigeration and waste treatment. Utility equipment is usually located outside the battery limit and may supply several processes. The cost of steam, electricity, and refrigeration depend mainly on fuel costs. Water, which is an increasingly important utility, is used both as a coolant and a process fluid. Cooling water is obtained from reservoirs, rivers, lakes, or even cooling tower. Process water quality depends on the needs of the process and may be filtered water, softened, de-mineralized cooling-tower water, condensate, distilled, and boiler feed water.

Compressed air is mainly used to operate pneumatic instruments and control valves. Air is also used in aerobic fermentations in biological waste treatment.

Refrigeration is needed when the required temperature is below the cooling water temperature. Refrigeration is also used when the material being processed is sensitive to high-temperatures.

Fuel costs have a major impact on utility costs and will have an even greater impact in the future. The hike of fuel price encourages the improvement of energy efficiency for processes.

2.3.3.5 Labor

Chemical plants require several types of labor. There is a direct labor, which is the operating labor needed to operate the plant, and maintenance labor who maintain the processes. There is also indirect labor, needed to operate and maintain facilities and services.

2.3.3.6 Plant maintenance

Maintenance costs consist of materials, labor and supervision. Although maintenance cost increases as a plant ages, economical estimates assume an average value for the life of the plant. The maintenance costs vary from 3% to 6% of the fixed capital cost per year [16]. Usually, an average value of 4.5% which consists of 60% labor and 40% materials is used.

2.3.3.7 Operating supplies

Supplies which are not raw materials or maintenance supplies, are considered as operating supplies. The examples are custodial supplies, safety items, tools, column packing, and uniforms. The cost of operating supplies will vary from 0.5 to 1% of the fixed capital cost per year [16]. Average value of 0.75% is used.

2.3.3.8 Quality control

Chemicals must meet certain specifications to be salable. Thus, analysis of process streams must be regularly made to determine product quality. Although there is a trend toward on-line analysis, samples of the process streams must still be taken to check

instrument performance. Also, there are still many analyses that cannot be made on-line. Peters and Timmerhaus [14], the cost of quality control varies from 10 to 20% of operating labor.

2.3.4 Indirect Costs

Indirect costs are costs incurred not directly related to the production rate and consist of fixed and plant overhead costs.

2.3.4.1 Fixed costs

The production rate will vary to economic condition accordingly, during the life of a plant, but depreciation, property taxes, insurance, and rent are independent of the production rate and will remain constant.

2.3.4.2 Depreciation

Depreciation can be evaluated from these aspects [17];

- i. a cost of operation
- ii. a tax allowance
- iii. a means of building up a fund to finance plant replacement
- iv. a measure of falling value

Value of a plant decreases with time because of wear and technical obsolescence. In a sense, a plant will be consumed to manufacture products. Depreciation determines the contribution of equipment cost to the production cost. There are several depreciation methods, which will not be discussed here.

An entire plant or individual equipment has three lives;

- i. economic life – occurs when a plant become obsolete
- ii. physical life – when a plant becomes too costly to maintain
- iii. tax life – fixed by the government

The plant life is usually ten to twenty years [13]. The depreciable capital cost includes all the costs incurred in building a plant up to the point where the plant is ready to produce, except land and site-development costs.

2.3.4.3 Plant overhead

Plant overhead is the cost of operating the services and facilities required by the productive unit. Also included are all the fringe benefits for direct as well as for indirect labor. It is common practice to include the fringe benefits of direct labor in the overhead rather than in direct costs.

2.3.5 General Costs

General costs are associated with management of a plant. Included within general costs are administrative, marketing, financing, and research and development costs. Table 3 divides general costs into various components. Marketing costs include technical service, sales, advertising and product distribution, consisting of packaging and shipping. Marketing cost vary from 5 to 22% of the production cost.

The interest rate on borrowed capital has increased considerably in the past. Usually, corporations and individuals will borrow capital when interest rates become favorable.

Finally, the process and product improvements are continuously being sought. Thus, the cost of research and development must be added to the production cost. Research and development varies from 3.6 to 8% of the production cost and average value of 5.8% is usually used.

CHAPTER 3: METHODOLOGY

3.1 Methodology

The research uses I2SI framework in Figure 1 to achieve its objectives. Integrated inherent safety index (I2SI) as in Equation (6) comprises of two main indices: a hazard index (HI) and inherent safety potential index (ISPI). The hazard index is a measure of the damage potential of the process after taking into account the process and hazard control measures. The inherent safety potential index, accounts for the applicability of the inherent safety principles (or guidewords) to the process. The HI and ISPI are combined to yield a value of the integrated inherent safety index ; $I2SI = \frac{ISPI}{HI}$ (6)

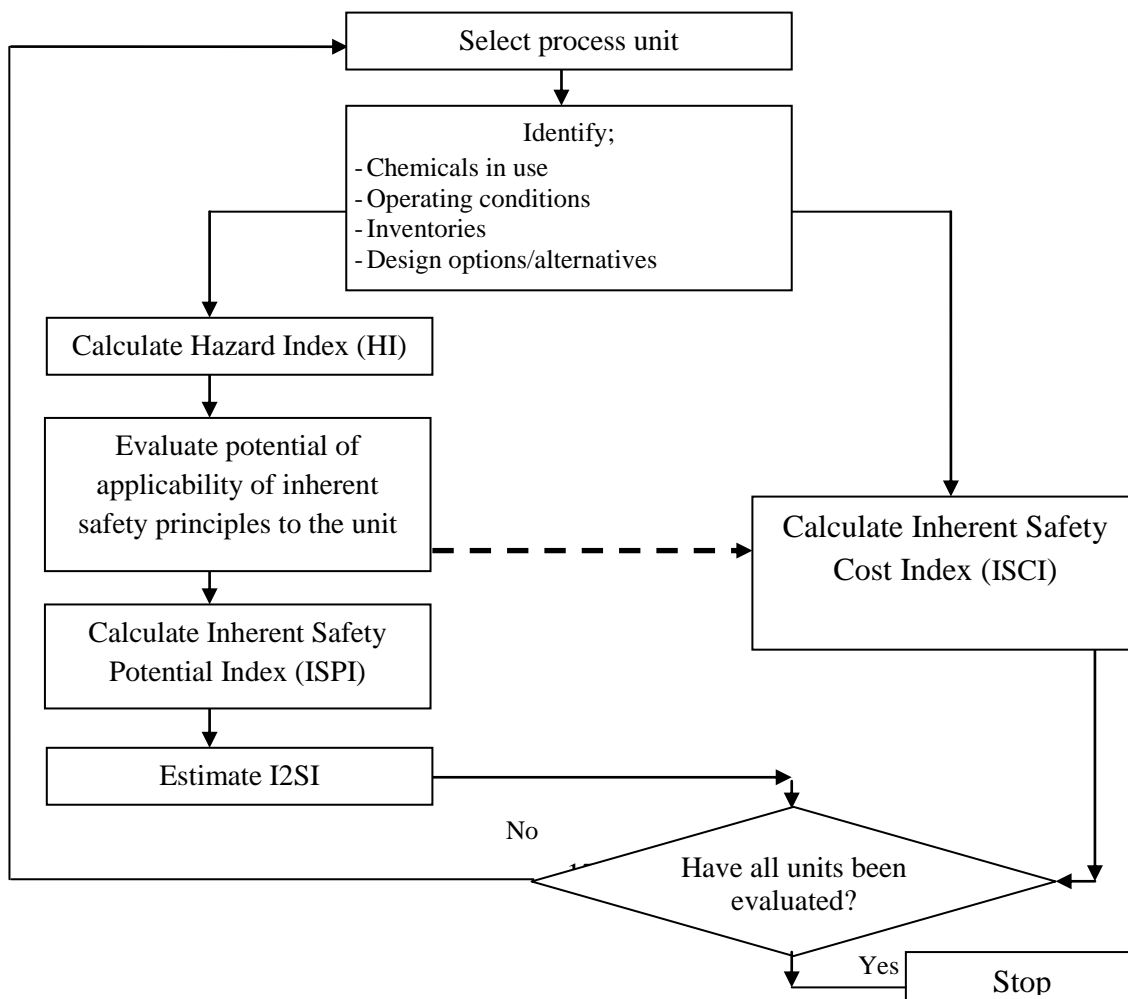


Figure 1 I2SI conceptual framework

Suitable process unit is selected. Data on chemicals in use, operating conditions and inventories is gathered. Hazard index (HI) is calculated by estimating damage radii (DR1 and DR2) and damage index (DI) by using SWeHI method. Process and hazard control index (PHCI₁) is also estimated to determine HI. HI is calculated by using Equation (7).

$$HI = \frac{DI}{PHCI_1} \quad (7)$$

Equation (8) shows inherent safety potential index (ISPI) is calculated by estimating inherent safety index (ISI) and process and hazard control index (PHCI₂) after implementing inherent safety principles.

$$ISPI = \frac{ISI}{PHCI_2} \quad (8)$$

The inherent safety cost index is determined by calculating the estimated loss, C_{loss} , conventional safety cost, $C_{convSafety}$ and inherent safety cost $C_{inhSafety}$. Conventional safety cost index (CSCI) and inherent safety cost index (ISCI) are determined by dividing conventional safety cost, $C_{convSafety}$ and inherent safety cost $C_{inhSafety}$ respectively with estimated loss, C_{loss} .

3.1.1 Conventional safety cost index (CSCI)

The conventional safety cost index (CSCI) is computed by Equation (9);

$$CSCI = \frac{C_{ConvSafety}}{C_{Loss}} \quad (9)$$

The numerator, $C_{ConvSafety}$, is the sum of the costs of process control measures and add-on (end-of-pipe) safety measures as in Equation (10).

$$C_{ConvSafety} = C_{Control} + C_{Add-on} \quad (10)$$

3.1.1.1 Process control measure costs

The cost of process control measures may be calculated by Equation (11);

$$C_{Control} = \sum_{i=1}^n N \times C_i \quad (11)$$

where C_i represents the cost of a given process control measure implemented N times, and n is the total number of control systems implemented. The cost of individual control measures may be taken from Table 4. To better represent the survey data, cost is subdivided into three different categories according to the severity of operating conditions.

- i) Class A: Process system/component operating in a normal capacity/normal severity, and requiring a conventional control system; for example, control measures for steam pipes, liquid chemicals, etc.
- ii) Class B: Process system operating under high capacity/hazardous chemical/severe operating conditions, and requiring an advanced control system; for example, control measures for pressurized gases, flammable liquids, high gas/liquid flowrates, steam, etc.
- iii) Class C: Process system operating under very high capacity/highly hazardous chemical/extremely severe operating conditions, and requiring an advanced control system; for example, control measures for liquefied gases, flammable gases, high gas/liquid flowrates, steam, handling fine dusts, etc.

Control system	Cost (000\$)		
	Class A	Class B	Class C

Control system	Cost (000\$)		
	Class A	Class B	Class C
Pressure control	2-4	4-9	9-15
Temperature control	1-3	3-6	6-12
Flow control	3-6	6-11	11-18
Level control	2-5	5-9	9-12
pH control	1-3	3-6	6-12
Additional control system (density control, concentration control, etc.)	2-5	5-11	11-19

Table 4 Classification of process control measure costs

3.1.1.2 Add-on safety measure costs

In a manner similar to the process control measure costs, the cost of add-on safety measures may be estimated by Equation (12) ;

$$C_{Add-on} = \sum_{j=1}^n N \times C_j \quad (12)$$

where C_j represents the cost of a given add-on safety measure implemented N times, and n is the total number of add-on safety systems implemented.

Control system	Cost (000\$) of one unit		
	Class A	Class B	Class C
Alarms	0.5-1.5	2-4	4-11
Detectors	2-3.5	4-8	9-20
Firefighting equipment	6-10	10-20	21-30
Blastwall	5-9	10-16	16-25
Sprinkling system	3-5	5-15	15-25
Inert gas blanketing system	4-10	10-17	18-30
Fire resistance wall	4-8	9-15	15-30
Other safety measures	3-7	8-14	14-32

Table 5 Classification of add-on safety measure costs

3.1.1.3 Calculating C_{loss}

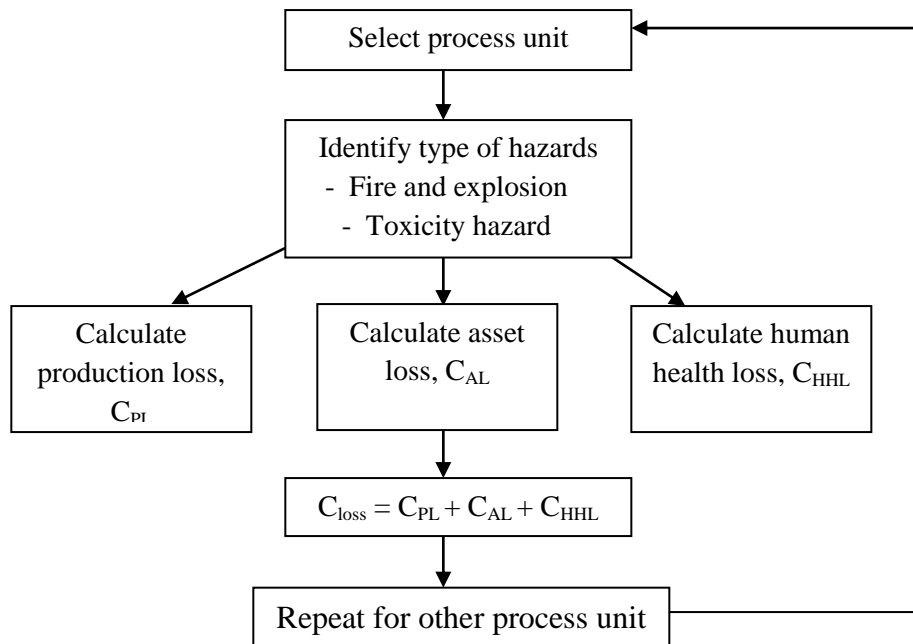


Figure 2 Simplified procedure to calculate C_{loss}

3.1.1.3.1 Production loss

For a given scenario, the production loss is calculated based on production hours loss multiplied by the cost of the each production hour. The value can be obtained via Equation (13).

$$C_{PL} = \text{Likely downtime (hours)} \times \text{Production value (\$/hour)} \quad (13)$$

3.1.1.3.2 Asset loss

Incidents (scenarios) involving fire, explosion or other similar events may cause loss of physical assets, such as damage to property, loss of equipment, etc. Asset loss may be simply calculated by using Equation (14):

$$C_{AL} = \text{Asset density (\$/area)} \times \text{Damage area} \quad (14)$$

3.1.1.3.3 Human health loss

For a given scenario, human health loss is calculated in terms of the number of fatalities/injuries and the costs associated with fatality and/or injury as shown in Equation (15);

$$C_{HHL} = \text{Damage area} \times \text{Population density (people/area)} \times \text{Cost of fatality/injury(\$)} \quad (15)$$

While the value of a human life is immeasurable, it is possible to employ indicators such as insurance costs, rehabilitation costs, worker compensation rates, etc.

CHAPTER 4: RESULTS AND DISCUSSION

4.1 Application of I2SI to ethylbenzene case study

To demonstrate the efficacy of the proposed indexing system we are visiting the ethylbenzene production case study. The chemistry of ethylbenzene manufacture via benzene-ethylene alkylation is straightforward:



Three different technologies are used; Friedel-Crafts technology which uses aluminium chloride (AlCl_3) as catalyst, Alkar process, and Mobil Badger. The raw materials used for ethylbenzene production are mainly ethylene and benzene.

Most of ethylbenzene manufacturer throughout the world uses low pressure liquid phase reaction processes which employ Friedel-Crafts chemistry and AlCl_3 as the catalyst. Some process technologies use the AlCl_3 -catalyzed route are Dow Chemical, Monsanto/Lummus, and Union Carbide Co./ Badger.

Alkar process introduced by Universal Oil Products uses a high-pressure process utilizing a solid fixed-bed catalyst, BF_3 on $\gamma\text{-Al}_2\text{O}_3$ [18]. The advantages it gives were reduced corrosion relative to AlCl_3 processes and the ability to operate using refinery streams containing relatively low ethylene contents as opposed to AlCl_3 processes which operated on pure 100% ethylene streams. This process found application primarily in small-scale plant, less than 200 MM lb/yr, although there were at least two large world scale plant, more than 500 MM lb/year outside of United States.

Other fixed-bed vapor-phase processes have been reported in the literature which used solid zeolite catalyst [19-22]. Zeolite catalysts were very active for benzene-ethylene alkylation but somehow they exhibit rapid aging which make them unsuitable for a

commercial process. Mobil Oil Corp. and the Badger Co. introduced a fixed-bed vapor phase process utilizing a new zeolite catalyst which had been demonstrated on a small commercial size unit (40 MM lb/year) [23]. The first world scale (1000 MM lb/year) was streamered in 1980 by American Hoechst Corp. at Bayport, Texas.

The advantages for the process were elimination of corrosion problems related to AlCl_3 process, nonpolluting effluents, alkylation and transalkylation conducted in the same reactor, higher energy efficiency by recovery of the exothermic heat of reaction, and process simplification brought about by the small size and number of vessels in the alkylation sector. In a later publication[24], the process was demonstrated using a dilute ethylene feed stream obtained from a treated fluid catalytic cracker off-gas. Presently, the Mobil/Badger ethylbenzene processe and the Monsanto-Lummus process appear to be the most economically attractive for manufacturing ethylbenzene.

The present world capacity for ethylbenzene is reported to be 13 to 14 million metric tons per year, with 40% of that capacity being in North America. 90% of the capacity comes from AlCl_3 process with Union Carbide Co./Badger processes being the predominant technology and accounting for about 25% of AlCl_3 processes.

4.1.1 AlCl_3 process

Polyalkylated and heavier aromatic materials are produced as by-products and require recycling to a separate transalkylation reactor. The amount of polyalkylated products can be reduced by increasing the benzene/ethylene in the feed in excess of the stoichiometric amount. The alkylation and transalkylation are carried out in separate reactors because the reaction rate for alkylation is much faster than that for transalkylation so that optimal process operation requires different operating conditions for the two reactions.

Minor amounts of side reactions have been reported, such as cracking and polymerization that result in the production of small amounts of a tarry residue. Optimal combination of operating conditions will not only depend upon the alkylated product but will also involve an optimization of the downstream process equipment such as distillation towers.

A modern liquid phase AlCl_3 alkylation process is divided into three sections: reaction section, catalyst disposal section and purification section. The exothermic heat of reaction of the alkylation reaction is recovered in the form of low-pressure steam. Because of the composition of the main reaction streams, corrosion-resistant materials of construction are necessary for the alkylation and transalkylation reactors. The product of the reaction section is then passes to catalyst disposal section. The AlCl_3 catalyst is removed from the hydrocarbon product by water washing and acid neutralization steps, and is either recovered by or sent to waste disposal. The third section, the purification section separates the hydrocarbon reaction products into the ethylbenzene product, benzene recycle and polyalkylated aromatic species (normally referred as polyethylbenzenes) which is recycled and residue. Overall, the process operates at 100% conversion of ethylene and reported yields of about 98 to 99 mol% based upon both ethylene and benzene feed.

Typical reaction conditions for etylbenzene manufacture via AlCl_3 alkylation are listed in Table 6.

Alkylation:		Transalkylation:	
Reaction temperature	300-350°F	Reaction temperature	300-350°F
Reaction pressure	70-150 lb/in. ² gauge	Reaction pressure	70-150 lb/in. ² gauge
Benzene/ethylene, mol/mol	1.5-2.5		
AlCl_3 /ethylene, mol/mol	0.0010-0.0025		

Table 6 Operating conditions for AlCl_3 process

4.1.2 Alkar process

The Alkar process, is a high-pressure fixed-bed process that uses BF_3 supported on $\gamma\text{-Al}_2\text{O}_3$ as the catalyst. The process offered the advantages of reduced corrosion when compared to AlCl_3 process, the ability to use dilute ethylene streams containing less than 10% ethylene which are available in many refineries, and a very high purity ethylbenzene product. In addition, the process offered greater simplicity since a catalyst recovery system, required in AlCl_3 alkylation, was not necessary. Nevertheless, commercial experience has shown that extensive waste treatment facilities are also required for the Alkar process.

The process can be divided into two sections, reaction section and product purification or separation section. The reaction section includes the benzene-ethylene alkylation reactor, the benzene dehydration column, a gas scrubber to remove aromatics from the effluent reactor gases, and the benzene recovery system. The purification section includes the benzene, ethylbenzene, and polyethylbenzene recovery columns and the transalkylation reactor. The purpose of the separate transalkylation and alkylation reactors is that, as in the case of AlCl_3 alkylation, the optimal operating conditions for alkylation and transalkylation differ because of different reaction rates.

The process flow starts with the dehydration of fresh and recycled benzene. Because the Alkar process utilizes a relatively small amount of adsorbed BF_3 in the catalyst, benzene and ethylene feeds must be bone dry to prevent removal of BF_3 catalyst by reaction with water. The dehydrated benzene is then combined with the fresh ethylene stream which is co-fed with the BF_3 make-up catalyst. The mixture is passed through the fixed-bed alkylation reactor. The reactor effluent is then passed through a two-stage flash recovery system in which the gaseous effluent is sent to a scrubber to remove all traces of aromatics while the main liquid product from the first flash vessel is sent to the separation section and a minor amount of liquid product from the second stage is recycled to the alkylation reactor. The gas scrubber also treats gaseous streams from the

benzene recovery system and the transalkylation system. The main liquid product from the alkylation reactor passes to a benzene recovery column where the benzene is taken overhead and then to a sorption column, containing a CaF_2 -charcoal mass, to remove traces of BF_3 before being recycled to the benzene dehydration column. The bottoms products from the benzene recovery column contains mainly ethylbenzene and polyethylbenzenes and is fed to the ethylbenzene recovery column where the ethylbenzene product is taken overhead. The bottoms product from the ethylbenzene columns is split. The major portion is sent back and used as the absorber liquid in the effluent gas scrubber while the remainder is sent to another column to remove the heavier alkylaromatics and then sent to the transalkylation reactor. The feed to the transalkylation reactor is composed of a benzene stream from the benzene dehydration column, the overhead product from the polyethylbenzene column, and a mixed benzene-polyethylbenzene stream from the effluent gas scrubber.

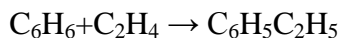
Although the Alkar process can use the cheaper dilute ethylene streams, considerable purification of the stream is necessary before it can be utilized since sulfur compounds, CO, and water, usually found in refinery gas streams, will poison the BF_3 catalyst. Like the AlCl_3 processes, the Alkar process operates at essentially 100% ethylene conversion and 99+% yields on both ethylene and benzene feed. Typical reaction conditions for ethylbenzene manufacture via Alkar process are listed in Table 7.

Alkylation:		Transalkylation:	
Reaction temperature	200-300°F	Reaction temperature	350-450°F
Reaction pressure	~500 lb/in. ² gauge	Reaction pressure	~400 lb/in. ² gauge
Benzene/ethylene, mol/mol	5-10		
AlCl_3 /ethylene, mol/mol	0.0005-0.002		

Table 7 Reaction conditions for Alkar process

4.1.3 Mobil/Badger process

The Mobil/Badger process is the most recent fixed bed, high-pressure, vapor-phase process to be introduced. It promotes the same overall alkylation chemistry:



but the mechanism, which is catalyzed by a zeolite catalyst, proceeds through a carbonium ion or carbonium ion-like mechanism which activates the olefin, ethylene, to make an adsorbed electrophilic species which is readily attacked by the aromatic species, benzene. This electrophilic species more readily undergoes oligomerization and subsequent cracking than the ethylene-catalyst complex of the Friedel-Crafts process. Hence alkylated aromatic species, not usually found in Friedel-Crafts processes, are formed, but these materials can be recycled to a steady state so that there is little or no net production and they do not occur in amounts that affect the purity of the ethylbenzene product.

Some of the proposed advantages of the Mobil/Badger process are the nonpolluting nature of the effluent and product streams, process simplicity not requiring a catalyst recovery section or separate transalkylation reactor, and because of the temperature and pressure of operation, 750-850°F, 200-300 lb/in.² gauge, >90% of the net process-heat input and exothermic heat of reaction can be recovered as medium- and low-pressure steam.

Like the Alkar process, the Mobil/Badger can process both pure ethylene feed and a dilute ethylene feed stream. Unlike the Alkar process, the catalyst in the Mobil/Badger process is relatively insensitive to many of the components that commonly occur in dilute ethylene streams: therefore, the high level of purification necessary for processes utilizing Friedel-Crafts catalysts is not required for the Mobil/Badger process. The main treatment of such dilute streams for the Mobil/Badger process is to remove C₃ and higher olefins which will alkylate and cause a yield loss in all processes.

The Mobil/Badger process is divided into two sections: the reaction section and a purification section. The reaction section contains two parallel, multibed reactors. The parallel reactors are required to allow regeneration of the catalyst without interrupting production. The catalyst becomes deactivated due to the deposition of carbonaceous material and requires regeneration after every 2 to 4 weeks of on-stream operation. The multiple-bed reactor design with interbed quench by reactants controls the adiabatic temperature rise in each bed and hence allows operation in a narrow optimal temperature range where cycle life and catalyst selectivity can be optimized.

Since transalkylation of polyethylbenzenes can be conducted at the same operating conditions as alkylation in the Mobil/Badger process, the recycle polyethylbenzene stream is combined with the recycle benzene and a fresh benzene stream and co-fed to the reaction section where both reactions are conducted simultaneously in a single reactor at conditions close to thermodynamic equilibrium. As was previously stated, the reaction mechanism over the zeolite catalyst produces other alkylaromatics, mainly in the C₈ and C₉ range. These materials are recycled in the polyethylbenzene stream to a steady state so that there is essentially no net production of these materials in the process.

The second section, the purification section recovers unreacted benzene for recycle to the reaction section. The bottoms product from the benzene recovery columns is further fractionated to produce an ethylbenzene product and polyethylbenzene recycle stream. A small aromatic residue stream is removed and used for fuel. The net process heat input and heat of reaction are recovered as low- and medium-pressure steam in the prefractionator condenser as well as the purification section condenser. Typical reaction conditions for the manufacture of ethylbenzene via the zeolite-catalyzed Mobil/Badger process are listed in Table 8.

Alkylation and transalkylation:	
Reaction temperature	750-850°F
Reaction pressure	200-400 lb/in. ² gauge
Benzene/ethylene, mol/mol	5-20
Ethylene weight hourly space velocity	2-10 lb/h/lb of catalyst

Table 8 Reaction conditions for Mobil/Badger process

4.2 Results and discussions

4.2.1 Option A (AlCl₃ process)

Intermediate and final results from the I2SI computations for the different units of this option are presented in Table 9.

Main process steps/units	DI	PHC I1	ISI	PH CI2	HI=DI/PHCI1	ISPI=ISI/PHCI2	I2SI=ISP I/HI
Dryer	141.507	38	14.2681	38	3.72387	0.37548	0.10083
Reactor I	141.449	55	14.2681	55	2.57180	0.25942	0.10087
Distillation column I	141.447	37	11.43	41	3.82289	0.27878	0.07292
Distillation column II	141.554	49	11.1722	42	2.88886	0.26600	0.09208
Distillation column III	141.507	44	10	45	3.21607	0.22222	0.06910
Reactor II	141.530	52	22.4975	44	2.72173	0.51131	0.18786

Main process steps/units	Closs(\$)	CconvSafety(\$)	CinhSafety (\$)	ISCI=CinhSafety/Closs	CSCI=CconvSafety/Closs	Closs(\$) with IS
Dryer	1.41E+07	6.70E+04	5.52E+04	0.00391	0.00475	7.06E+06
Reactor I	3.77E+07	1.07E+05	5.82E+04	0.00154	0.00284	1.89E+07
Distillation column I	1.41E+07	1.07E+05	5.82E+04	0.00413	0.00759	7.06E+06
Distillation column II	1.65E+07	8.70E+04	8.62E+04	0.00522	0.00527	8.27E+06
Distillation column III	4.25E+04	1.07E+05	5.82E+04	1.36941	2.51765	2.12E+04
Reactor II	4.77E+06	7.70E+04	5.77E+04	0.01210	0.01614	2.39E+06
	8.72E+07	5.52E+05	3.74E+05			4.37E+07

Table 9 Integrated inherent safety index and cost indices for option A (AlCl₃ process)

Intermediate and final results from the I2SI computations for the different units of this option are presented in Table 9. It can be seen that none of the units is having an I2SI value greater than unity. An I2SI value which is greater than unity represents that the value Hazard Index (HI) is lesser than the Inherent Safety Potential Index (ISPI). The reactor has low value of I2SI, mainly due to its high hazard index and comparatively low inherent safety potential index. The high index is due to a large volume of chemical used and catalyst handling (AlCl_3 catalyst).

Cost indices (CSCI and ISCI) which are greater than unity signifying that the costs of the safety measures on these units are higher than the expected losses. Distillation column III has value greater than unity for both CSCI and ISCI (1.37 and 2.52 respectively) because of its low expected loss. Considering a cost index value of unity as a balance condition where safety costs equal the expected loss, most of the process units in option A are performing in a suboptimal manner from a financial perspective.

4.2.2 Option B(Alkar process)

Intermediate and final results from the I2SI computations for the different units of this option are presented in Table 10.

Main process steps/units	DI	PHCI1	ISI	PHCI2	HI=DI/PHCI1	ISPI=ISI/PHCI2	I2SI=ISPI/HI
Reactor I	141.513	52	11.380	43	2.72140	0.26465	0.09725
Dryer	141.493	38	10.177	38	3.72350	0.26782	0.07193
Distillation column I	141.447	37	11.430	41	3.82289	0.27878	0.07292
Distillation column II	141.554	49	11.172	42	2.88886	0.26600	0.09208
Distillation column III	141.507	44	10.000	45	3.21607	0.22222	0.06910
Reactor II	141.562	52	22.498	44	2.72235	0.51132	0.18782

Main process steps/units	Closs(\$)	CconvSafety(\$)	CinhSafety (\$)	ISCI=CinhSafety/Closs	CSCI=CconvSafety/Closs	Closs(\$) with IS
Reactor I	1.94E+05	8.90E+04	4.72E+04	0.24339	0.45876	9.69E+04
Dryer	1.94E+05	6.70E+04	5.52E+04	0.28454	0.34536	9.69E+04
Distillation column I	1.41E+07	1.07E+05	5.82E+04	0.00413	0.00759	7.06E+06
Distillation column II	1.65E+07	8.70E+04	8.62E+04	0.00522	0.00527	8.27E+06
Distillation column III	4.25E+04	1.07E+05	5.82E+04	1.36941	2.51765	2.12E+04
Reactor II	4.77E+06	7.70E+04	5.77E+04	0.01210	0.01614	2.39E+06
	3.58E+07	5.34E+05	3.63E+05			1.79E+07

Table 10 Integrated inherent safety index and cost indices for option B (Alkar process)

The results of the I2SI computations for option B are presented in Table 10. The I2SI value for reactor is still low because of high temperature usage in the main reactor. The temperature used is 120°C. Hazard index for reactor II is the highest, because of high operating temperature than the main reactor temperature is used (200°C). Analyzing other process units individually, it may be observed that the process hazard control indices are approximately the same, signifying that not much enhancement of inherent safety has been made.

As in option A, distillation column III has value greater than unity for both CSCI and ISCI (1.37 and 2.52 respectively) because of its low expected loss. From the indices, it can be concluded that most of the process units in option B are not performing in optimal manner from a financial perspective.

4.2.3 Option C (Mobil/Badger process)

Intermediate and final results from the I2SI computations for the different units of this option are presented in Table 11.

Main process steps/units	DI	PHCI1	ISI	PHCI2	HI=DI/PHCI1	ISPI=ISI/PHCI2	I2SI=ISPI/HI
Reactor	141.456	55	14.268	55	2.57193	0.25942	0.10087
Distillation column I	141.447	37	11.430	41	3.82289	0.27878	0.07292
Distillation column II	141.554	49	11.172	42	2.88886	0.26600	0.09208
Distillation column III	141.507	44	10.000	45	3.21607	0.22222	0.06910

Main process steps/units	Closs(\$)	CconvSafety(\$)	CinhSafety (\$)	ISCI=CinhSafety/Closs	CSCI=CconvSafety/Closs	Closs(\$) with IS
Reactor	3.77E+07	1.07E+05	5.82E+04	0.00154	0.00284	1.89E+07
Distillation column I	1.41E+07	1.07E+05	5.82E+04	0.00413	0.00759	7.06E+06
Distillation column II	1.65E+07	8.70E+04	8.62E+04	0.00522	0.00527	8.27E+06
Distillation column III	4.25E+04	1.07E+05	5.82E+04	2.74528	5.04717	2.12E+04
	6.83E+07	4.08E+05	2.61E+05			3.43E+07

Table 11 Integrated inherent safety index and cost indices for option C (Mobil/Badger process)

The results of the I2SI computations for option C are presented in Table 11. The I2SI value for reactor is high because of high temperature usage in the reactor (430°C). Eventhough the number of process units is lesser in option C, but because of operating conditions need for operations, none of the process units achieved a value of I2SI

greater than unity. Non-optimal application of inherent safety is still lacking in this process.

The same case goes for cost indices. Only distillation column III has a value of CSCI (2.75) and ISCI(5.05) greater than unity showing that the expected loss is comparatively low than the safety measures costs. All of the process units in this option is not financially preferable.

The followings are the cost comparison summary that has been developed for the case study.

Option	Technology	in million \$			
		Expected loss without IS	Expected loss with IS	CconvSafety	CinhSafety
A	Friedel-Craft	87.21	43.7	0.552	0.3737
B	Alkar	35.8	17.9	0.534	0.363
C	Mobil/Badger	68.3	34.3	0.408	0.261

Table 12 Cost comparison between Friedel-Craft, Alkar and Mobil/Badger technology

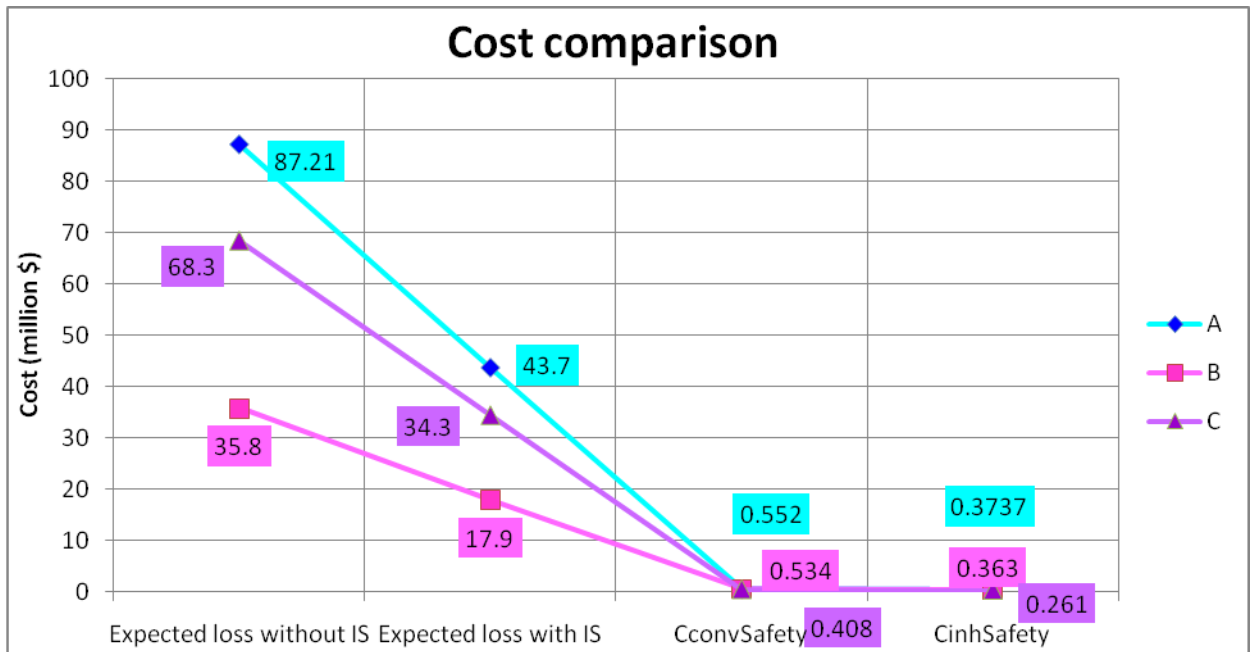


Figure 3 Cost comparison for Friedel-Craft, Alkar and Mobil/Badger technology

Figure 3 shows the comparison for expected loss without inherent safety, expected loss with inherent safety, conventional safety cost and also inherent safety cost. The expected loss cost is higher when inherent safety is not applied. Applying inherent safety in the process consequently reduce the probability of accident occurrence, therefore, reducing expected loss for the whole plant. It can be concluded that even though the cost for conventional safety is slightly higher than the cost for inherent safety, but the expected loss is still high.

In reality, implementing inherent safety in the process route could increase the inherent safety cost depending on the process conditions (more hazardous conditions require higher cost for inherent safety). Theoretically, the inherent safety cost will be higher but the cost of losses will be less because the probability of accidents happen is reduced. When accident occurrence can be reduced, the damage radii and damage index will also be smaller. Thus, the expected loss will be lower. Over time, higher cost of inherent safety equipment will be compensated with lesser loss to the company.

As Alkar process posses the least value for all parameters (expected loss without inherent safety, expected loss with inherent safety, conventional safety cost, inherent safety cost), therefore option B (Alkar process) is the most economical yet safer process for ethylbenzene production.

CHAPTER 5: CONCLUSION AND RECOMMENDATIONS

5.1 Conclusion

Inherent safety principles should be implemented in the process design so that the probability of accident/injury happen can be reduced and directly reduces the cost of losses over the long run. Although the application for inherent safety will require higher cost than conventional control cost, but throughout the whole plant lifetime, lesser loss can be expected from the plant.

Referring back to the case study, Alkar process is the preferred process route as it is financially cheaper. Inherent safety principles should be implemented thoroughly in the process so that the I2SI value of Alkar process can be enhanced.

5.2 Recommendations

- The case study should be detail out more to obtain more accurate value. The parameters should be gathered carefully for each process route and major equipment.
- Include minor equipment in the case study evaluation. Having the minor equipment together in the evaluation will represents the overall process route, not partial of it.
- The safest process route can be evaluated by developing case study which uses different chemicals as raw material to produce the same output. Different chemical and thermodynamics properties will apparently gives clear differentiation between the process alternatives.

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APPENDIXES

APPENDIX A I2SI SPREADSHEET (SAMPLE)

APPENDIX B GANTT CHART OF FINAL YEAR PROJECT

Activity/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20		
FYP II briefing							MID SEMESTER BREAK															
Project work commences																						
Concept review-inherent safety (IS) principles and IS index																						
Review of methodology																						
Submission of Progress Report 1					26/8																	
Project work continues																						
Revise methodology																						
Case study development																						
Poster Exhibition/Pre-EDX/Progress Reporting												12/10										
Submission of Progress report 2												15/10										
EDX													18/10									
Submission of Final report (CD softcopy & softbound)															8/11							
Final Oral presentation																					29/11-10/12	
Submission of hardbound copy																						17/12