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Development of a Risk Based Inherent Safety Index Using an Integrated Approach

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Keywords: risk based safety index, inherently safer design, life cycle approach, petrochemical process

Abstract

The growing demand for petrochemical products and the implementation of new process technologies have made the petrochemical plants more complex; therefore, it becomes more challenging to manage the risk. Traditionally, additional layers of protection were added to prevent incidents, which further adds complexity to the existing process. Inherently safer design aims at managing the risk from the design stage of petrochemical plants, which eliminates the hazard in the process rather than control the risk during operation. When designing a new plant or modifying an existing plant, a safety index system will be helpful to assess the risk level of various options effectively. This can be achieved by considering the inherently safer design principles, *i.e.*, elimination, substitution, moderation, and simplification. In this work, a novel safety index system was developed to cover the life cycle of a process design, which includes the research stage, process development stage, and engineering design stage. This safety index will be used to evaluate the risk level of petrochemical facilities by comparing toxic, flammable, explosive, runaway reaction, dust and physical explosion risks and identify the areas where inherently safer design principles can be used to improve the process. A case study on ethanol synthesis process will be presented for the validation of the index system developed.

1 Introduction

With a growing population, an increasing number of petrochemical facilities are being built with larger capacity and more complexity, which pose a great risk to assets, community and environment. As the same time, the general public demands a higher standard for safety performance of petrochemical industries. The add-on barriers are traditionally used to manage the risk at operation stage, but it has proven to be ineffective and costly. The concept of inherent safe was introduced by Trevor Kletz twenty years ago with the expression of “What You Don't Have Can't Leak” [1]. The value of inherently safer design is recognized with time by all stakeholders. Recently, the proposed revision of several major process safety regulations mandate inherently safer technology in the process design. However, an effective tool is needed to evaluate and compare inherent safety of alternative technologies.

Process safety strategies can be implemented at different stages of the process design life cycle. The earlier efforts are made to improve safety, the better the outcome is in terms of safety performance and cost. The effectiveness of these strategies needs to be evaluated to ensure a desirable safety level and guide the continuous efforts for further improvement. Previous safety index systems exist to assess process safety level; however, safety indices that cover all stages of process design are limited. This work aims to develop a safety index system for inherently safer design through a life cycle approach.

2 Methodology

2.1 Model framework

The primary objective here is to develop a safety index system to evaluate risk levels of process technologies, aiming to select a safer alternative and identify opportunities for inherently safer design. This index system is based on a life cycle approach of process design, including research stage, process development stage, and engineering design stage. In each stage this novel index system will have different focuses, namely chemical safety, equipment safety and engineering control measures, as shown in Figure 1. Stage 1 includes analysis of chemical hazards. Stage 2 considers the failure rates of major equipment. Stage 3 considers the contribution of engineering safeguards to improve safety. These engineering safeguards can be either passive or active to reduce the risk of a potential hazard scenario. Having defined the scope and the approach of the index system, the overall framework is presented in Figure 1. It is important to highlight that the analysis of safety index can be stopped at any one of the three stages depending on the need of required study and available information. The result of stage 1 is a hazard index, because only chemical information is considered. From stage 2, the analysis result is a risk index with consideration of equipment failure rates. The only exception of the stage-by-stage approach is the reaction risk index, because it covers all three stages if picked for analysis.

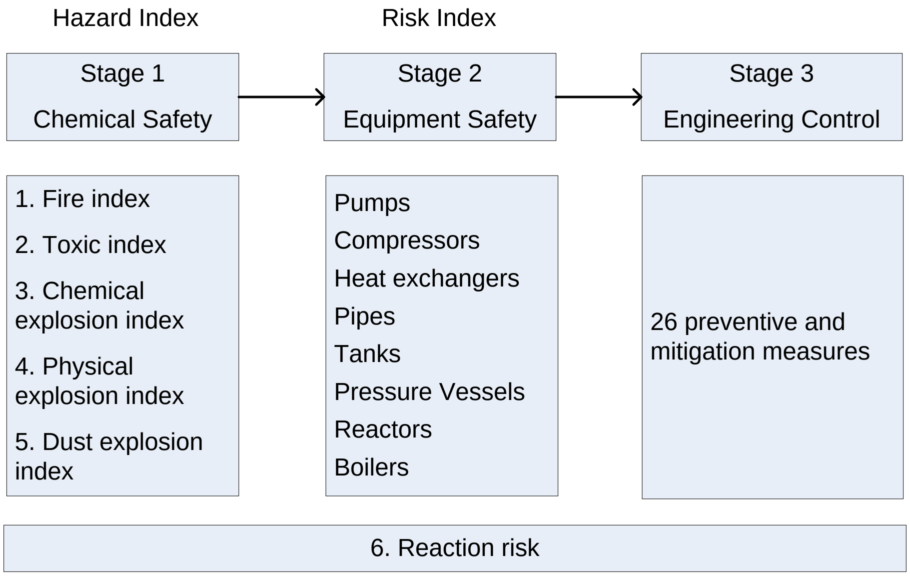


Figure 1 The framework of the safety index system

In Stage 1, the chemical compounds are selected to analyze the chemical safety. All the parameters necessary for the model calculations of stage 1 will be explained later. Then the incident scenarios are generated for the chemicals chosen, together with specified process and release conditions: pressure, temperature, leak hole size and quantity of release. The process conditions together with the chemical properties are used to generate the hazard index of stage 1. This index carries information on the consequence of the chemical release. Different scenarios may be generated using different conditions and compared, and alternative processes with different chemical routes can be as well compared at this stage for chemical safety.

For the second stage, the process equipment is included in the analysis by considering the failure rates. The combination of failure rate with hazard index from stage 1 allows one to obtain a risk index at stage 2. This notion comes from the definition of risk itself where risk is a function of both probability and consequence [2]. For this stage, the equipment is selected and combined with the release conditions, *i.e.* hole size, a failure rate is obtained based on the Offshore and Onshore Reliability Data (OREDA). A risk matrix is developed to determine the risk index with both hazard index from stage 1 and equipment failure rate.

At stage 3, engineering barriers are considered to control the risk based on the information of previous stages, *i.e.*, chemical safety and equipment safety. Each barrier will be applicable depending on its nature, to one of the indices. Also, the barriers have an active or passive nature and can be categorized between preventive and mitigative. Once the barrier is chosen, the Probability of Failure on Demand (PFD) of the barrier is used for the calculation. For the final stage, the probability of risk is obtained by combining the PFDs of safety barriers and equipment failure rate. The probability modified was calculated as:

$$Updated\ Failure\ Frequency\ \left[\frac{1}{year}\right] = Failure\ Rate\ \left[\frac{1}{year}\right] * PFD$$

Following the same procedure, to assess the final risk index from Stage 3, the updated failure frequency probability calculated is combined with the hazard index from Stage 1 to obtain a risk index according to a matrix system developed in this work.

2.2 Tool development

On behalf of user-friendly application, an interactive tool was developed using Microsoft Excel Visual Basic for Applications TM. The tool was developed as an attempt to automatize the process of preliminary analysis and application of inherently safer design principle to a series of scenarios. The tool allows the user to apply the three stages to different scenarios depending on design and process specifications. Thus, the objective is to be able to compare and select the inherently safer design that is being considered for the analysis.

The tool was developed using Microsoft Excel 32-bit version, due to the known broad use this software has in different industries and levels within the companies. The tool intends to be a user-friendly and easy-to-understand Excel spreadsheet that uses Macros as the form of interaction with the user. Macros are used as the simplification and automation tool within Excel that allows one to easily input the parameters needed and select the scenarios

Therefore, the use of macros will allow the end user to interact with the safety index calculations throughout the different stages of process design lifecycle, and will also allow a better reporting method for the scenarios selected. The purpose of the tool includes but is not limited to the automated method of calculation for further comparison of different design scenarios with the goal of selecting the inherently safer process.

As now the tool designed takes into account the individual scenarios. This means that no consideration for mixtures or combination of equipment is considered. Each scenario is constrained to consider a single chemical, a single equipment, and a single barrier. This does not mean that complex processes cannot be analyzed using the tool. Engineering expertise is required to compare a complex chemical process by considering all possible scenarios. A node analysis is needed to specify the analysis being developed [3].

3 Model development

3.1 Stage 1

3.1.1 Simulation-based indices: explosivity, flammability, toxicity

In this section, the method of calculating safety indices at three different stages is explained. As previously described, the three initial indices, flammability, explosivity and toxicity, were developed using a simulation-based approach. The indices were developed in three steps. First, generation of data; second, model generation; and finally, normalization and index generation.

Generation of data

In order to accurately represent consequence data for flammable, explosive and toxic scenarios, a series of consequence analysis scenarios were generated. The consequence analysis data was produced in the form of consequence distance using a commonly used consequence distance modeling software. Using PHAST, simulation of 17 chemicals was conducted to provide results to training Neural Network in the second step. The list of chemicals used in PHAST simulation were selected based on the following criteria:

- Chemical involved in the incidents provided by the incident database from Sinopec. Also, an analysis was performed to compare the incidents from Sinopec and those from the United States Chemical Safety Board.
- Chemicals with their properties cover a full range of various hazards. For example, chemicals with NFPA ranking from 1 to 4 in each NFPA category.
- Chemicals exist in the PHAST database.

Table 1 shows the number of scenarios generated for each consequence type.

Table 1 Total number of simulations for each hazard

Index	Number of Scenarios simulated
Flammability	3,046
Explosivity	40,800
Toxicity	3,069

Model generation

Neural Network models were developed based on the chemical parameters and corresponding PHAST consequence results. The neural network models were developed by selecting a series of parameters for each index. A parametric analysis was conducted to choose parameters showing a strong influence on consequence results of each hazard.

Figure 2 shows the R value of the training, testing and all data for the fire index. The training, validation, and testing data were randomly selected from the PHAST consequence data. 80% of the raw data were randomly selected for training. 10% of data were randomly selected for validation. The remaining 10% of data were selected for testing. The Bayesian Regularization algorithm has been used and is intended to make sure the results of the training data fit the test and validation data. When R =1, it is a perfect fit. So the R values of 0.988, 0.986, and 0.977 for all data for fire, explosion and toxicity are considered good results.

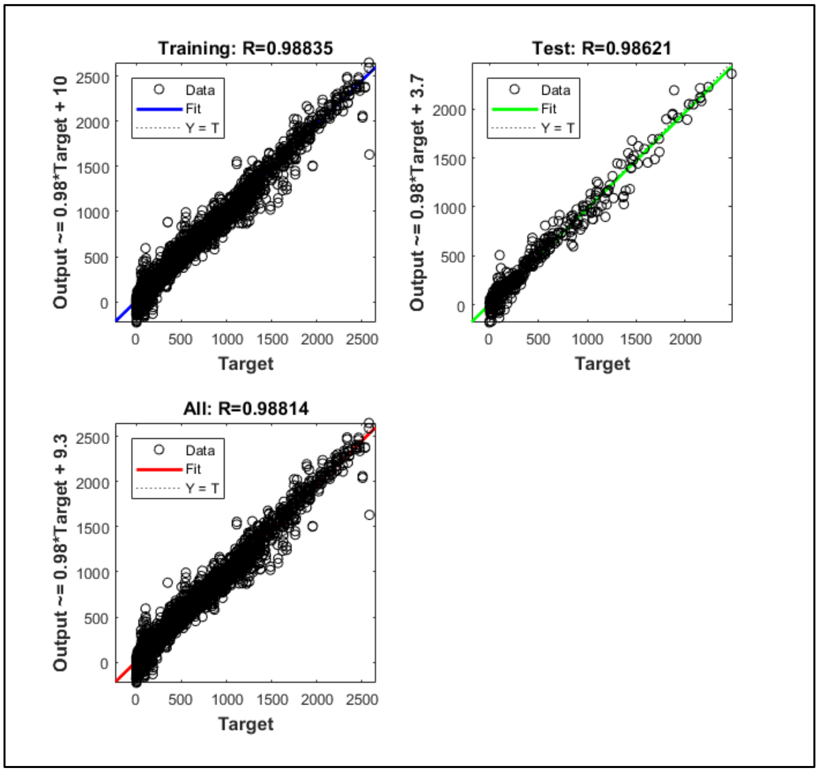


Figure 2 Regression results of the neural network simulation of flammability (12.5 kW/m²)

Normalization and index generation

i) Interpolation: The safety indices for toxic release, fire, and explosion are neural network models fit to PHAST simulation results. As all models, the neural network models developed in this study have limitations. Generally, these models can calculate relative safety levels using a number of input parameters; however, there are cases that result in negative neural network values since neural network method only provides the best model to fit existing data points. Efforts were made to reduce negative results, but it is not able to eliminate all negative values in this work. In order to make sense of the index results, additional efforts were taken to adjust the negative results using interpolation method.

The interpolation method uses three parameters from the simulation-based indices. All three indices have Pressure and Temperature as main parameters. The third parameter for interpolation purposes is IDLH for the toxic index, Heat of Combustion for fire index and Flammability Range (UFL-LFL) for explosion index. Pressure and temperature information will be adjusted using Table 2 to determine the range of interpolation. Take pressure, for example, if the input pressure is 50 psi, the adjusted pressure is 100 psi and the pressure range index is 2. Similarly, the temperature range index can be determined. Therefore, the interpolation range can be determined if these two range indices are combined. After the range is selected, the interpolated result is finally determined by the third parameter. Given an input value of the third parameter, the interpolated result will be the PHAST result with the closest value to the input of the third parameter. The interpolation method applies only if the neural network models provide invalid values. Otherwise, the normal Neural Network results will be used for each index.

Table 2 Ranges for interpolation for the parameters of Pressure and temperature

Range Index	Temperature Input [ºC]	Temperature Range [ºC]	Input Pressure [psi]	Pressure Range [psi]
1	-25 or below	-50	1 or below	1
2	-24-24	0	2-150	100
3	25-200	100	151-300	200
4	201-400	300	301-500	400
5	401-600	500	501-700	600
6	601 or above	700	701-900	800
7			901 or above	1000

ii) Normalization: Mapping the consequence results into 0-100 was done using the normalization method. This helps to adjust values measured on different scales to a common scale. For the flammable, toxic, and explosion hazards, the simulated results range on different scales, which is difficult for the users to tell the severity of the consequences from the results. Therefore, it is necessary to do the normalization to compare the results under same common scale (0-100), wherein 0 indicates least hazardous and 100 indicates most hazardous. The following equation is used:

$$Index\ [0-100] = \frac{Consequence\ Distance\ (m)}{\text{Normalization Factor}(m)} * 100$$

Once the consequence distances were calculated from Neural Network model, a normalization factor was needed. The normalization factor needs to take into account the distribution of the data for each hazard in order to establish an index system with a consistent ranking scale.

For the simulation-based indices (*i.e.* flammability, explosivity, and toxicity), the normalization factor was taken from the previously filtered data of PHAST simulation software. Different values were used to see which accounted for the majority of the data. Values for 25, 50, 75 and 100 percentiles of consequence distance were used. With a few trials, 75 percentile was found to be a reasonable value according to the distribution of the data; therefore it was selected as the normalization factor. The 75 percentile values are 600 m, 2400 m, and 800 m for flammability, toxicity and explosivity, respectively. If the results from Neural Network model is higher than the normalization factor, the index value is capped at100.

3.1.2 Adopted indices: dust explosion, physical explosion, and reaction

The indices of dust explosion [4], physical explosion [5] and reaction [6] are adopted from literature with some modifications to ensure a consistent ranking system.

3.2 Stage 2

The Stage 2 of the inherent safety index focuses on various equipment that is commonly used in a process plant. The equipment was shortlisted based on operations taking place in the petrochemical industry. The hazard identification included the collection of the failure rates of the equipment to analyze.

A major assumption made for developing risk index for various equipment in Stage 2 relates to the release type. Full release, a consistent release at normal operating pressure, is the one selected in this study because it fits the desired characteristics and scope of this study. The full release is defined as to be consistent with flow through the defined hole, beginning at the normal operating pressure, and continuing until controlled by emergency shut-down and blowdown if present and operable, or inventory exhaustion.

3.2.1 Methodology

The steps followed to calculate the risk index associated with equipment in Stage 2 are:

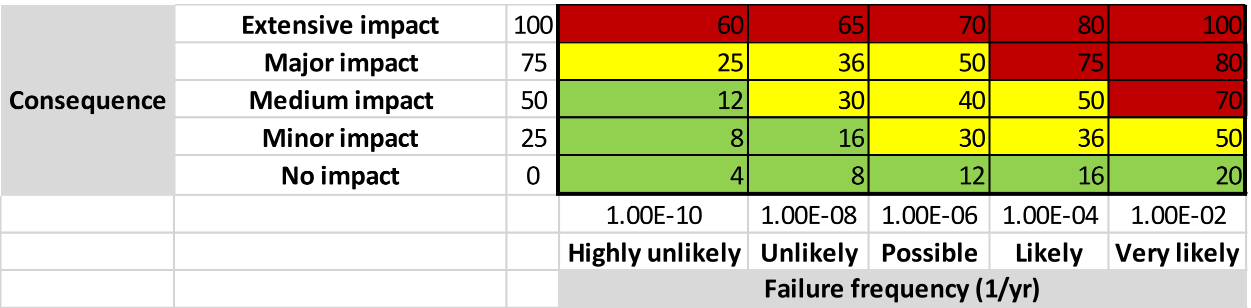
a) Various equipment in the process plant were classified into four major classifications: mechanical; electrical; bulk transport and movable storage based on the UK HSE HID CI5 document [7]. These were further sub-classified into vessels; components; pipework; pipelines and containers. The details are presented in Table 3. Among different classes of equipment, different sub-types were also selected for the analysis. For example, Heat Exchanger is an equipment that is used for the physical operation of heating or cooling. There were three different types of heat exchanger selected, these include shell and tube, plate and air-cooled heat exchanger. Different types were also considered for other equipment wherever possible.
b) Five different hole sizes are considered for risk index determinations. These hole sizes are 25 mm, 50 mm, 500 mm, 750 mm, 1000 mm. The above hole sizes were selected to represent a range of scenarios from small, medium to large releases.
c) The next step is to assign the right failure frequencies of equipment and these depend on two main parameters: Hole Size and Release Size. The dependencies of failure rate on various equipment are shown in Table 3.
d) Based on the step above, failure rate frequencies are assigned to various scenarios using the OGP failure rate database [8].

Table 3 Dependency of failure rate for various equipment

Type of Equipment	**Sub-classification**	**Dependency of failure rate**
Physical Operations		
Heat Exchanger	Shell and tube	Hole Diameter, Release size
	Plate heat exchanger	Hole Diameter, Release size
	Air-cooled	Hole Diameter, Release size
Pipes	Fixed pipe network	Hole Diameter, pipe length
Pumps	Centrifugal pump	Hole Diameter, Release Size
	Reciprocating	Hole Diameter, Release Size
Compressor	Centrifugal	Hole Diameter, Release Size
Pressure Vessels	Large vessels	Release Size
Small and medium atmospheric tanks	Flammable content	Release Size
Chemical Operations		
Reactors	General	Hole Diameter, type of release
	Non-Flammable content	Release Size
Utilities		
Boilers		Release Size

3.2.2 Index determination

Since the index of runaway reaction risk is a risk index, five sub-indices are combined with equipment failure rate to generate the risk indices, including fire; explosion; toxic release; dust explosion and physical explosion. This makes use of the risk matrix shown in Figure 3.



Consequence	**Extensive impact**	100	60	65	70	80	100
	Major impact	75	25	36	50	75	80
	Medium impact	50	12	30	40	50	70
	Minor impact	25	8	16	30	36	50
	No impact	0	4	8	12	16	20
			1.00E-10	1.00E-08	1.00E-06	1.00E-04	1.00E-02
			Highly unlikely	**Unlikely**	**Possible**	**Likely**	**Very likely**
			Failure frequency (1/yr)				

Figure 3 Risk matrix for stage 2

3.3 Stage 3

The stage 3 of the safety index focuses on various safety controls or barriers that are commonly used in a process plant. These controls or barriers aid in reducing the probability of occurrence of process safety events and/or reducing the severity of the consequences. For the evaluation of risk index in Stage 3, the safety controls or barriers were shortlisted based on various process operations in petrochemical industry and experts' opinions. It is important to note that this list is a sample list and can be improved continuously by adding safeguards. The user may add more controls while carrying out the assessment based on the case study at hand.

3.3.1 Methodology

The steps followed as part of this methodology for evaluation of the Stage 3 index are: (i) list all the possible engineering controls in a process plant; (ii) classify the controls as active or passive controls; (iii) categorize the controls as preventive or mitigative controls based on the purpose, *i.e.*, whether the control/barrier is effective in reducing consequence or frequency; (iv) assign probability of failure on demand (PFD) value to each listed control (various sources *e.g.*, CCPS; OREDA database; IEC 61511); (v) calculate final sub-index value using the PFD mean value, after incorporating the barrier for risk reduction. This has been presented below as a flowchart in Figure 4.

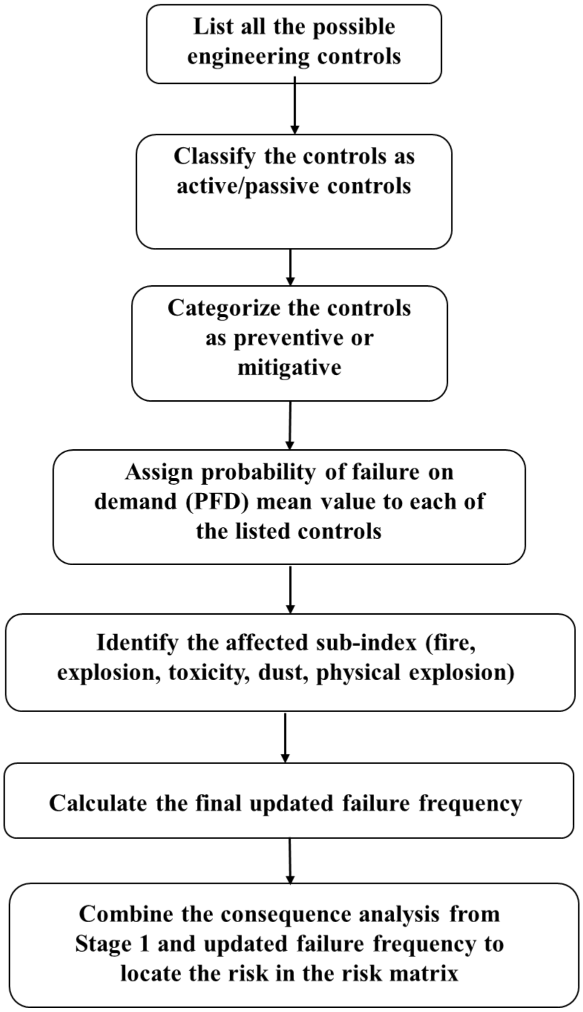
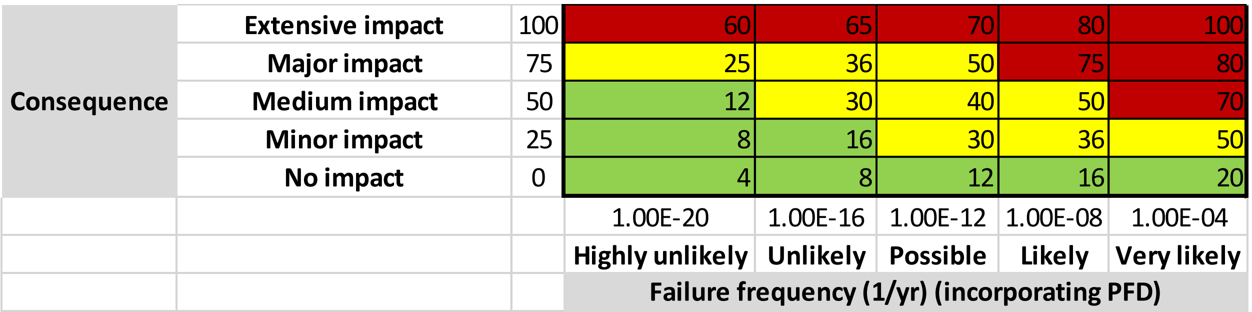


Figure 4 Stage 3 methodology

3.3.2 Index determination

For the incorporation of the impact of these controls to the final risk assessment, a method similar to Layer of Protection Analysis (LOPA) is followed. The failure probability values from Stage 2 are multiplied by the PFD of the selected controls or safeguards for the particular scenario to obtain the updated failure probability for Stage 3. Finally, a risk matrix was used to determine the risk index as shown in Figure 5.



Consequence	**Extensive impact**	100	60	65	70	80	100
	Major impact	75	25	36	50	75	80
	Medium impact	50	12	30	40	50	70
	Minor impact	25	8	16	30	36	50
	No impact	0	4	8	12	16	20
			1.00E-20	1.00E-16	1.00E-12	1.00E-08	1.00E-04
			Highly unlikely	**Unlikely**	**Possible**	**Likely**	**Very likely**
			Failure frequency (1/yr) (incorporating PFD)				

Figure 5 Risk matrix for stage 3

4 Case study

The case study aims to demonstrate the use of index system to identify a safer process and assist with the decision making. In the case study, two processes producing ethylene are selected: one is catalytic dehydration of bio-ethanol and the other is oxydehydrogenation of ethane [9].

Process 1 - Catalytic dehydration of bio-ethanol

The process of converting bio-ethanol to ethylene is shown in the Figure 6. The first step is to preheat the ethanol, which is then converted to the main product, ethylene, by the endothermic dehydration of ethanol. Since the reactor output contains some impurities, it must be subjected to a downstream purification step. Purification steps include water washing, caustic washing, absorption and drying to obtain the desired chemical grade ethylene. There are different kinds of design to complete the process. In this case study, the design of Petrobras, as shown in Figure 7 is chosen.

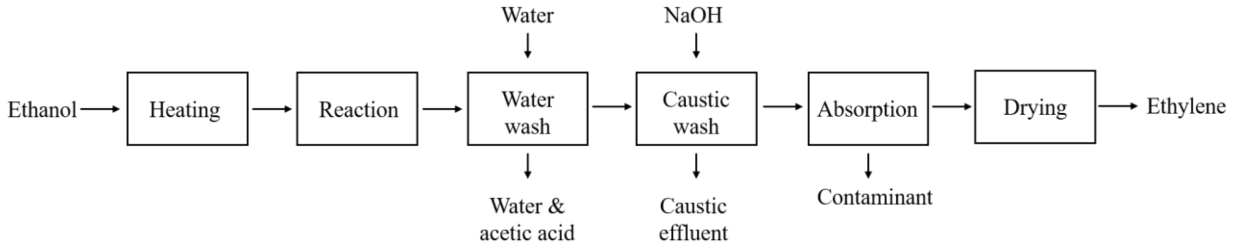


Figure 6 Conversion of bio-ethanol to ethylene via dehydration [9]

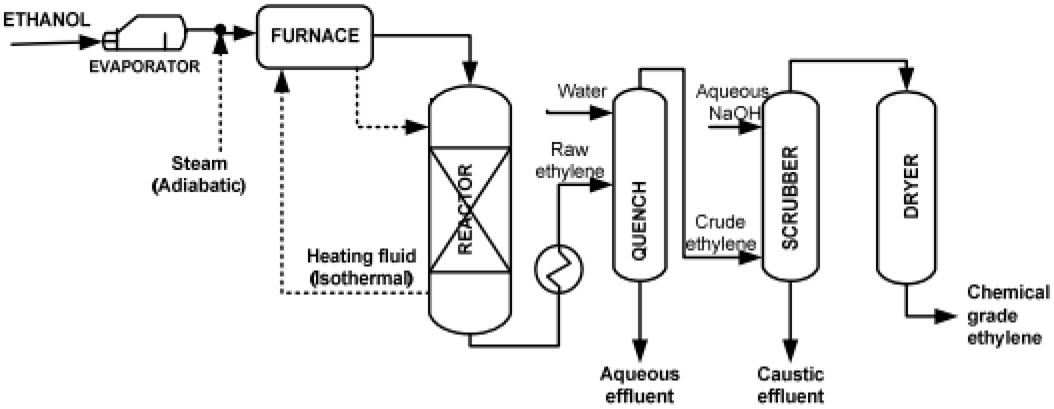


Figure 7 Simplified flow diagram of the Petrobras dehydration process [9]

Process 2 - Oxydehydrogenation of ethane

Figure 8 shows the process flow diagram designed by Union Carbide with its key conversion and separation steps. Figure 9 depicts the simplified flow diagram of the Union Carbide.

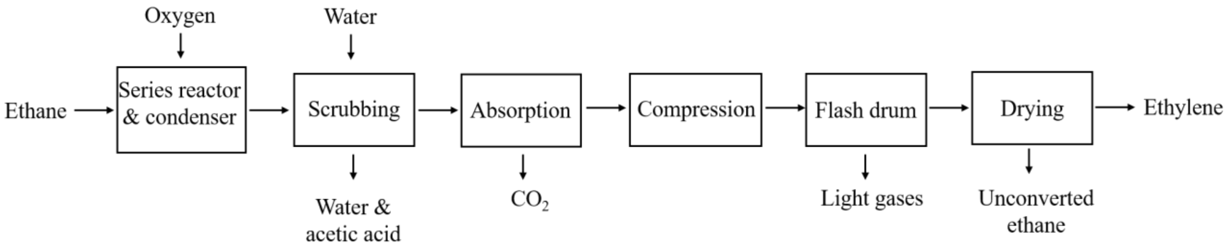


Figure 8 Block diagram of ethane to ethylene via oxydehydrogenation [9]

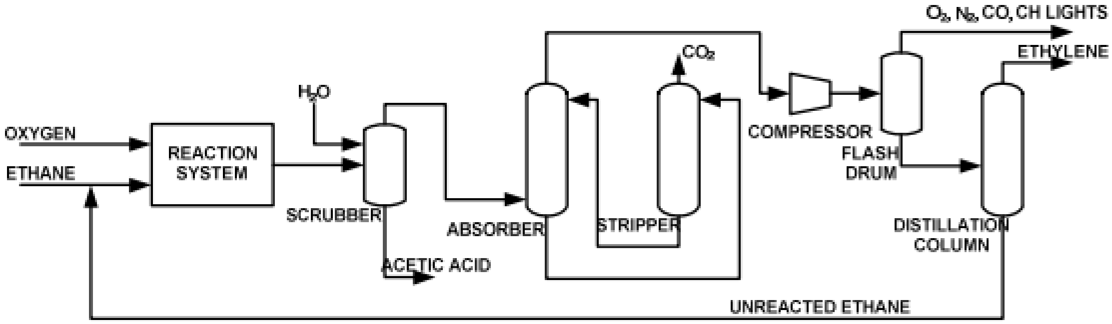


Figure 9 A simplified flow diagram adapted from the Union Carbide oxydehydrogenation process [9]

During this process, the ethane and oxygen feedstock supplied by the air separation unit are compressed, mixed and preheated before entering the reactor. The oxydehydrogenation reaction takes place in a series of three reactors in which ethane is introduced into the first reactor and oxygen is supplied in parallel (to each reactor inlet). At each reactor, the feed stream was preheated to about 250 °C and converted to ethylene in a free radical reaction at 300-400 °C.

The reacted product stream comprises ethylene, acetic acid, water, unreacted ethane, unreacted oxygen, gases produced by side reactions such as carbon monoxide and carbon dioxide, and other gases present in commercial ethane. The scrubber separates the remaining aqueous acetic acid and then the gas from the scrubber removes the carbon dioxide through the amine adsorption system. Next, the gas stream is compressed and introduced into the distillation column. The top product of the distillation is ethylene, with ethane and other gases in the bottom. Ethane from the distillation column is recycled back to the reaction system.

The chemicals involved in these two processes are summarized in Table 4.

Table 4 Substances involved in the two processes

Pathway	**Dehydration process**	**Oxydehydrogenation process**
Raw material	Ethanol	Ethane
Main reaction	$2CH_3CH_2OH \rightarrow H_2C{=}CH_2 + 2H_2O + CH_3CHO$ (by-product)	$CH_3CH_3 + 1/2O_2 \rightarrow H_2C{=}CH_2 + H_2O$
Desired product	Ethylene	Ethylene
Main by-product	Ethanol	Ethane, O_2
Other by-product	Acetaldehyde and Acetic acid	Acetic acid
Other by-products or gases		CO and CO_2

Given the chemicals and equipment involved in the two processes, the indices of flammability, toxicity and explosivity are selected for the analysis. The study includes major chemicals, equipment and fire detection as the control barriers. The result shows that the dehydration process is safer than oxydehydrogenation process in terms of flammability and explosivity indices, but not the toxicity index. Overall, the oxydehydrogenation process is safer.

5 Conclusions

In this work, a novel safety index system was developed to cover the life cycle of a process design, which includes research stage, process development stage, and engineering design stage. This safety index can be used to evaluate the risk level of petrochemical facilities by comparing toxic, flammable, explosive, runaway, dust and physical explosion risks and identify the areas where inherently safer design principles can be used to improve the process. A case study on ethanol synthesis process was conducted for the validation of the index system developed.

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