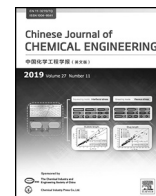




Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJChE

Article

Development of index system for inherently safer process design using an integrated approach☆

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ARTICLE INFO

Article history:

Received 7 November 2018

Received in revised form 3 July 2019

Accepted 16 July 2019

Available online 30 July 2019

Keywords:

Inherently safety

Chemical process safety

Integrated risk-based safety index

PHA/ST

Hydrogen dioxide

ABSTRACT

With a growing population, an increasing number of petrochemical facilities are built with larger capacity and more complexity, which pose a great risk to assets, community and environment. The value of inherently safer design is recognized with time by all stakeholders, and an effective tool is needed to evaluate and compare inherent safety of alternative technologies. This study developed a safety index to evaluate existing technologies for their safety levels and guide inherently safer design. The Integrated Risk-based Safety Index (IRSI) was developed based on a comprehensive review of petrochemical processes, incident cases from Sinopec and US Chemical Safety Board, and existing safety index systems. The IRSI included all major hazards, including fire, explosion, toxic release, dust explosion, physical explosion, and runaway. Also, the integrated life cycle approach considered chemical hazards, equipment failure rates and safety measures in this risk-based index. Advanced modeling techniques, PHAST simulation and Neural Network, were used in the development of three novel sub-indices in the projects, fire, explosion and toxic release. The index system could be easily incorporated into a user friendly tool for the ease of application. A case study of hydrogen dioxide was conducted using the IRSI, which showed its capability for evaluating the safety level of process facilities.

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1. Introduction

Industrial plants as well as the general public demand a higher standard for safety performance of facilities. The add-on barriers are traditionally used to manage the risk at operation stage, but it has been proved to be ineffective and costly in many cases. The concept of inherent safety was introduced by Trevor Kletz with the expression of 'What you don't have can't leak' [1,2]. The value of inherently safer design is recognized with time by all stakeholders in chemical industry, coal industry, environmental protection, transportation and even urban public safety. The realization of the inherently safer process design is a way to solve the safety problems of chemical process fundamentally, which is of great significance to avoid major safety accidents [3].

The most conventional and popular approach to qualitatively evaluate the hazards of a system is the Hazard and Operability method (HAZOP) [4]. However, HAZOP can only be implemented after the detailed design of the plant is available, and requires significant amount of time and effort [5]. The design of inherently safer processes has been arranged in four main categories: minimization or intensification,

substitution, moderation or attenuation, and simplification [6]. The methodologies in the literature are as follows: assigning scores or sub-indices for each parameter, and the final index is a weighted average of each sub-index given by expert opinions; correlating parameters to consequence of the process to give a consequence factor; correlating parameters to risk of the process with consequence factor, penalties and credit factors [7]. The outputs of the index can be as follows: single score to rank systems based on expert opinion, hazard radius in meters, based on which a qualitative ranking of the system is developed to help the comparative analysis, risk in terms of business loss, business interruption and fatalities as a comparative tool.

Safety indices have several degrees of details regarding the input required for their use, which means that different indices would be suitable for application depending on the state of development of process design [8]. The first safety index reported in the literature was developed by Dow in 1964, known as the Dow Fire & Explosion Index (F&EI); the index was based on the material properties and process conditions [9]. Dow's chemical and exposure index (C&EI) was the basis for the development of the Mond index by Lewis, which included the toxicity of the chemical [10]. A parallel development was the Dow Chemical & Exposure Index, which took into account the toxic exposure from chemicals. Both Dow F&EI and Dow C&EI were found to have ample use in the chemical industry. Khan and Abbasi developed the Hazard Identification and Ranking (HIRA), an index to overcome some of the

☆ Supported by the National Key Research and Development Program of China (2016YFB0301701) and National Natural Science Foundation of China (21606258).

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limitations of the Dow Fire & Explosion Index, because the material factor in Dow's index was considered as independent of the operating conditions and there was more dependence on expert opinions than that on the system properties [11]. Recently, a quantifying inherent safety methodology was developed based on the design stage under consideration using a quantification technique that utilized process data available during the specific stage of design [12]. An improved framework was proposed based on fuzzy logic using chemical properties, process data, and chemical accident databases [13].

From the several safety indices reported in the literature, a selection of representative indices can be applied at different stages of process design and the type of output obtained from their application. In existing safety index system, various parameters were collected based on different factors: inherent safety principles (intensification or minimization, substitution, moderation, and simplification), hazard classes (fire, explosion, toxic exposure, and common indirect factors), and industrial design phase (research stage, process development stage, engineering design stage, and in-service operation stage).

Although the proposed revision of several major process safety regulations mandates inherently safer technology in the process design, an effective tool is needed to evaluate and compare inherent safety of alternative technologies. Inherently safer process design based on analysis of the life cycle of a petrochemical manufacturing plant reveals a series of opportunities to ensure that it makes the greatest possible contribution to safety and the triple bottom line. At a number of key stages during the life cycle of a process, there are chances to make better, more informed decisions, and to make sure that their investments create the maximum value. These opportunities include: selecting the safer and most cost-effective process designs, optimizing the detailed design of the process, scheduling the availability of new capacity to coincide with demand 'up cycle', maintaining the plant at the safe optimum level during its lifetime, improving operational performance by increasing efficiency and removing bottlenecks. This study aims to develop a safety index system to evaluate safety levels of existing technologies and guide inherently safer design. Also, the safety index system could be easily incorporated into a user friendly tool for the application.

2. Development of Safety Index

This study took a life cycle approach to use information from different stages of process design in the development of a novel safety index system (shown in Fig. 1). Stage 1 included six major hazards. The

integrated method including Neural Network and PHAST simulation was used to develop fire, chemical explosion and toxic indices. The other three indices were adopted from literature. Stage 2 included the failure rates of major equipment, so that the safety index system was made as risk index covering both consequence and frequency. The safety index for reaction was a risk index taken from literature; therefore there was no need to consider equipment failure rates at stage 2. Stage 3 included the safety measures to reduce either consequence or frequency.

2.1. Stage 1 index - chemical safety

PHAST simulation of 17 chemicals was conducted to provide results to training neural network. The chemical list was selected based on the following criteria: chemical that is involved in typical incidents; chemicals with their properties covering all the range of the physical and chemical properties, and chemical indices, for example, chemical with the NFPA from 1 to 4 in each NFPA category; chemicals exist in the PHAST database [14]. The incident analysis was based on the CSB report about incidents in the U.S. and Sinopec database about the incidents in China. For incident analysis based on the CSB report, all the incident reports were looked through and 25 incidents (from 1998 to 2012) were selected. The Sinopec database has a list of 135 incidents that cover from year 1972 to 2011. All the incidents' information was summarized and a list of chemicals that were involved in the incidents was obtained.

Based on the chemical parameters of PHAST consequence results, a neural network model was developed. Fig. 2 shows the regression value (R) of the training, testing and all data, and the training, validation and testing data was randomly selected in the PHAST consequence data. 80% of the raw data was randomly selected for training, and 10% of data was randomly selected for validation and testing respectively. When $R = 1$, it is perfect fitting and the regression value 0.97717 for all data is a considerably good result.

Fig. 3 shows the regression value of the training, testing and all data for the neural network simulation of flammability. 80% of the raw data was randomly selected for training, and 10% of data was randomly selected for validation and testing respectively. The regression value 0.98814 for all is a considerably good result.

Fig. 4 shows the regression value of the training, testing and overall data for explosion. 80% of the raw data was randomly selected for training. 10% of data was randomly selected for validation. 10% of data was

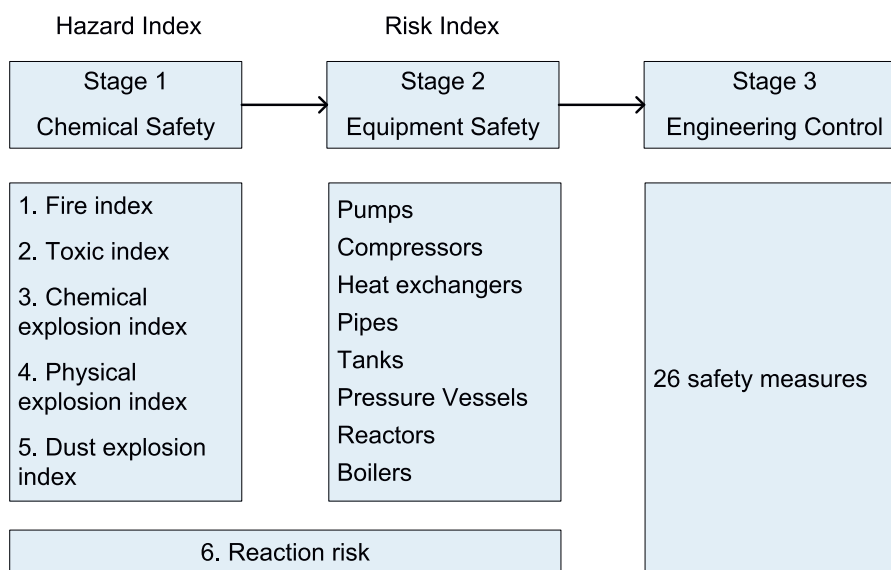


Fig. 1. The flow chart of index system development.

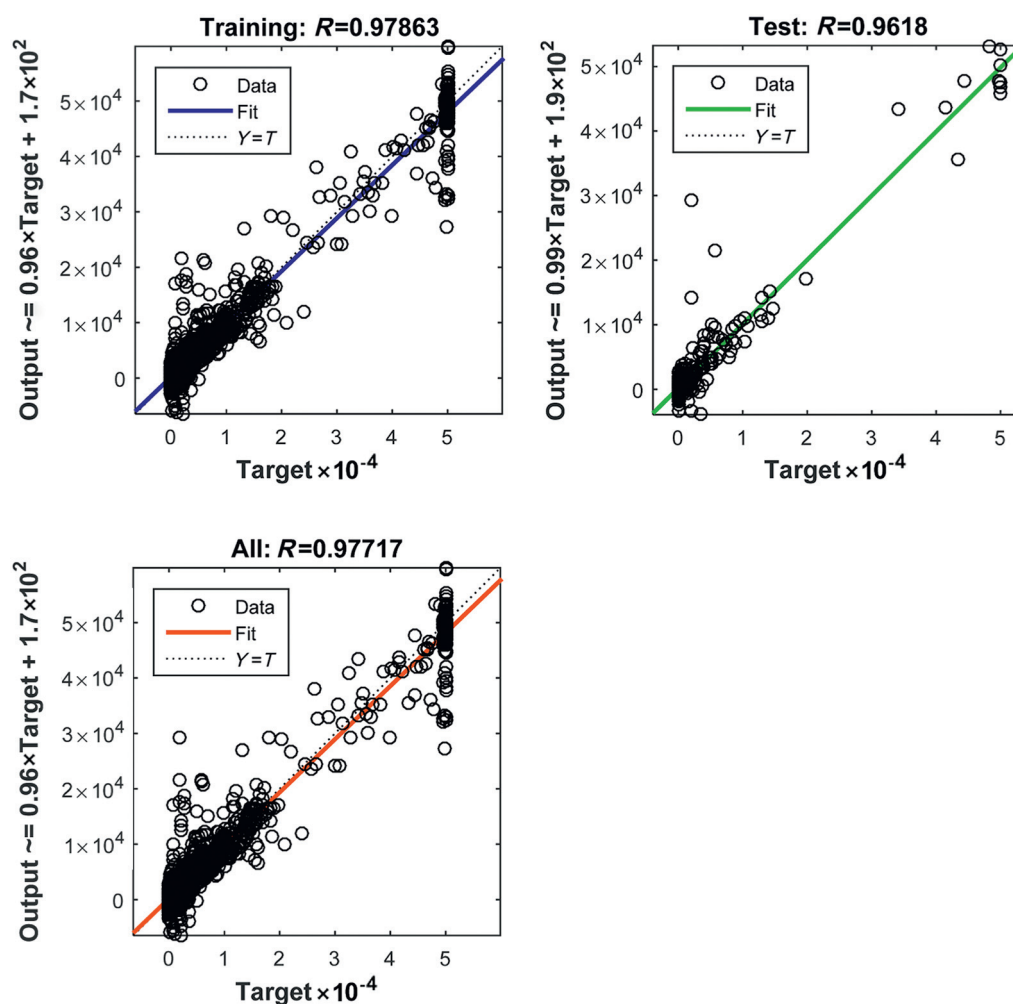


Fig. 2. The regression results of the neural network simulation of toxicity 0.01.

randomly selected for testing. The Bayesian Regularization algorithm was used to make sure the results of the training data fit the test and validation data. The regression value 0.98569 for all is a considerably good result.

Generally, the neural network models trained by PHAST simulation results can calculate relative safety levels using a number of input parameters; however, there are cases whose results of neural network are negative values. Additional efforts were also taken to adjust the negative results using interpolation method for reliable results.

The interpolation method uses three parameters for toxic index, fire index and explosion index. All three indices need pressure and temperature. The third parameter is IDLH for toxic index, Heat of Combustion for fire index and Flammability Range (UFL-LFL) for explosion index. Pressure and temperature information will be adjusted 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 a closest value to the input of the third parameter. The interpolation method will be adopted only if the neural network models provide negative

values. Otherwise, the normal neural network results will be used for each index (Tables 1 and 2).

The index for dust explosion mainly draws lessons from 'Dow's Fire & Explosion Index Hazard Classification Guide', and the index of physical explosion mainly depends on 'Multivariate hazard identification and ranking system' [15]. This physical explosion is represented in distance at which there is structural damage [11].

The runaway risk index for assessing exothermic runaway risk is described by Eq.1 [16].

$$RRI = \frac{1}{1.6} \sum_{j=1}^4 I_j \times \frac{1 + \sum \text{risk factors}}{1 + \sum \text{safety factors}} \quad (1)$$

I_j consists of Reactivity (Nr) (NFPA), Stability (St), Exothermic Enthalpy (Exo), and Energy Severity (ES). The ranges for each are given in Tables 3–5:

2.2. Stage 2 index - equipment safety

The stage 2 of the risk based inherent safety index focuses on various types of equipment that are commonly used in a process unit. Therefore, the stage 2 index could be named as Equipment Risk Index (ERI). The equipment was shortlisted based on typical operations in petrochemical industry; therefore identifying the risk of

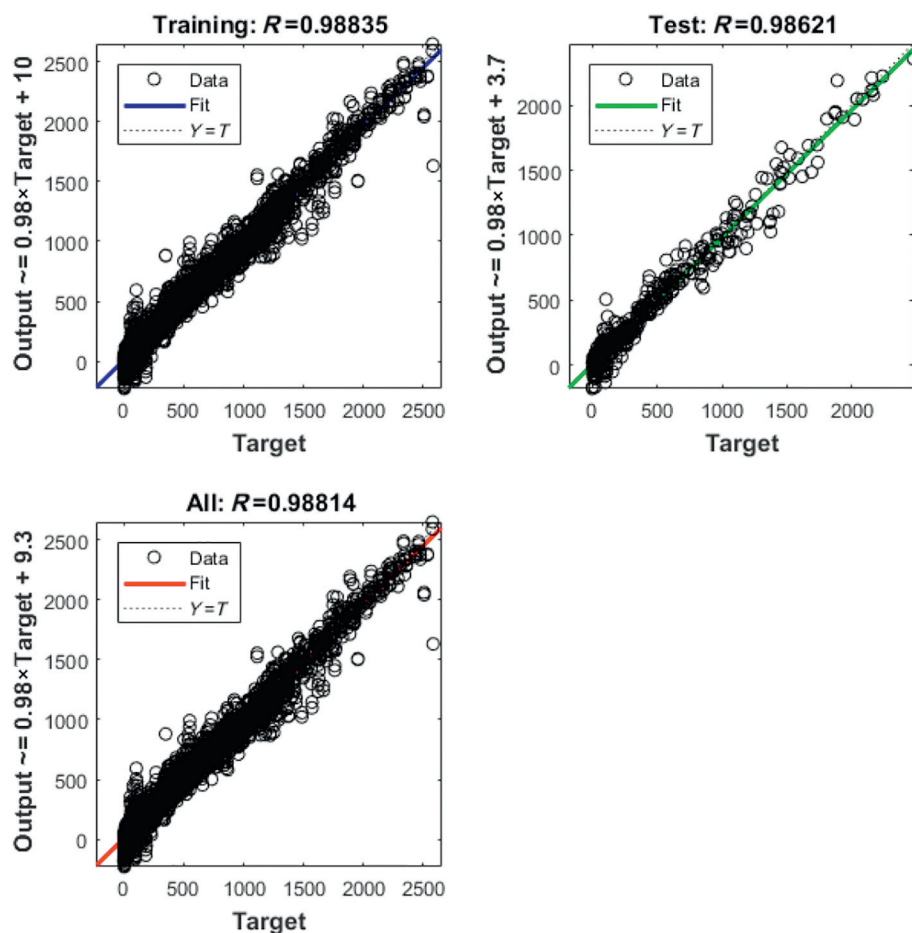


Fig. 3. The regression results of the neural network simulation of flammability ($12.5 \text{ kW} \cdot \text{m}^{-2}$).

failure for the equipment to develop the risk assessment. The hazard identification included the recollection of the failure frequency rates of the equipment to analyze. An exhaustive literature review was made in order to collect relevant information to assess the stage, and recognized risk assessment directories such as OGP and HSE were the key to establish this index [7,11,17]. The combination of consequence results obtained in stage 1 with the failure rate results determines the Risk Index for stage 2.

The following assumptions were made for developing the methodology for calculation of the risk index for various equipments in stage 2. Releases can be divided into three different types: limited releases (the release is isolated locally by human intervention), zero pressure releases (equipment normal zero operating pressure or depressurized) and full releases (consistent release at normal operating pressure). The last release type (full release) was selected in this study because it fits the desired characteristics and scope of this study. The full release type is assumed to be consistent with flow through the defined hole, beginning at the normal operating pressure, and continuing until controlled by emergency shut-down and blow down (if present and operable) or inventory exhaustion. This scenario is invariably modeled in any QRA (Quantitative Risk Analysis).

Various equipments in the process plant were classified into four major classifications: mechanical, electrical, bulk transport, and movable storage. These were further sub-classified into vessels, components, pipe work, pipelines and containers. The details are presented in Table 6. Among different classes of equipment, different sub-types

were also selected for the analysis. For example, heat exchanger is equipment that is used for physical operation of heating. There were three different types of heat exchanger selected, including shell and tube, plate, and air-cooled heat exchanger. Different types were also considered for other possible equipment.

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 equipments are shown in Table 7.

Based on the step above, failure rate frequencies are assigned to various scenarios using the OGP failure rate database. Five sub-indices are combined with equipment failure rate to generate the risk indices, including fire, explosion, toxic release, dust explosion, and physical explosion. The consequence in terms of distance from stage 1 is combined with failure rate of equipment to calculate the risk at stage 2, using 'Risk = Consequence Distance $\times$ Failure rate'. The results are mapped to a scale of 0–100 using a similar method as stage 1.

2.3. Stage 3 index - engineering control

The stage 3 of the risk based inherent safety index focuses on various safety controls and/or barriers that are commonly used in a process unit. These barriers or controls aid in reducing the probability of occurrence of process safety event and/or reducing the severity of the consequences. The controls or safety barriers were shortlisted based on various process operations in petrochemical industry and available

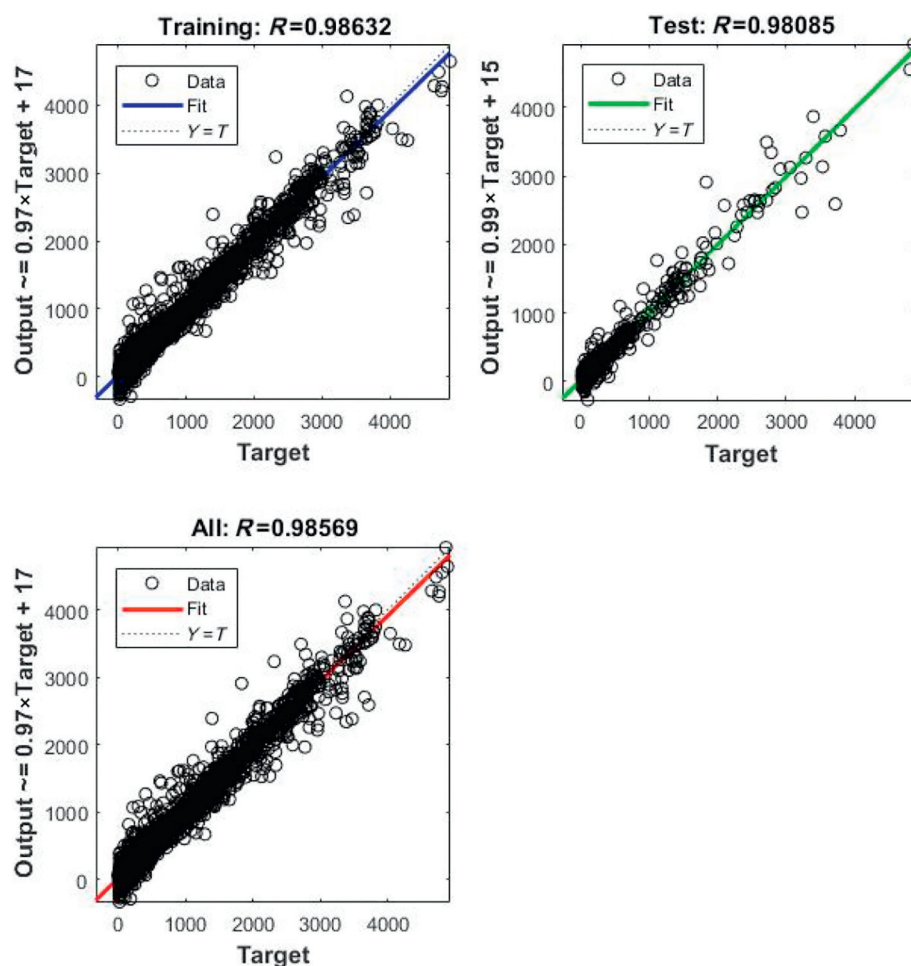


Fig. 4. The regression results of the neural network simulation of explosion (2 psi).

Table 1

Pressure range index

P/psi (1psi = 6.895 kPa)		
Input	Adjusted input	Range index
1 or below	1	1
2–150	100	2
151–300	200	3
301–500	400	4
501–700	600	5
701–900	800	6
901 or above	1000	7

Table 2

Temperature range index

T/°C		
Input	Adjusted input	Range index
–25 or below	–50	1
–24–24	0	2
25–200	100	3
201–400	300	4
401–600	500	5
601 or above	700	6

Table 3

Stability factor

(dT/dt) _{max} /°C·min ^{–1}	Adiabatic temp. rise, ΔT _{ad} /°C		
	>100	50–100	<50
<50	3	2	1
50–200	4	3	2
>200	4	4	3

Table 4

Exo score (1cal = 4.1868 J)

Heat released per unit mass/cal·g ^{–1}	Exothermic score
>300	4
300–100	3
100–20	2
<20	1

literature as well as experts' opinions. It is important to note that this list is a sample list and can be improved continuously. Researchers may add more controls while carrying out the assessment based on the case study at hand, which can be primarily categorized into process controls

and layers of protection/barriers (emergency shutdown, interlocks, sprinkler system). Following are the list of steps followed as part of this methodology:

1. To list all the possible engineering controls in a process plant.
2. To classify the controls as active or passive controls.
3. To categorize the controls as preventive or mitigate controls based on purpose *i.e.*, whether the control/barrier is effective in reducing

Table 5

ES: Energy Severity for various reaction types

Reaction type		Energy Severity value
Oxidation	Highly exothermic	4
Nitration	Highly exothermic	4
Halogenation	Highly exothermic	4
Diazotization	Highly exothermic	4
Hydrogenation	Highly exothermic	4
Thermal decomposition	Highly exothermic	4
Polymerization	Highly exothermic	4
Sulfonation	Exothermic	3
Condensation	Exothermic	3
Amination	Moderately exothermic	2
Esterification	Moderately exothermic	2
Methylation	Moderately exothermic	1
Alkylation	Moderately exothermic	1
Hydrolysis	Moderately exothermic	1
Salt formation	Moderately exothermic	1
Reduction	Low	0
Electrolysis	Low	0
Isomerization	Low	0
Cyclization	Low	0

consequence (which type of consequence- fire, vapor cloud explosion, toxic release, physical explosion or dust explosion) and frequency.

- To assign probability of failure on demand (PFD) value to each listed control (various sources *e.g.*, CCPS; OREDA database; IEC 61511 [18, 19])
- To calculate final sub-index value using the PFD mean value, after incorporating the barrier to help in risk reduction.

For the incorporation of impact of these controls to the final risk assessment, an evaluation similar to Layer of Protection Analysis (LOPA) is proposed. The stage 2 index value will be multiplied by the PFD of the selected controls for the particular scenario to arrive at the stage 3 index value. The details are shown in Table 8.

3. Case Study of Hydrogen Dioxide Process

The purpose of this case study is to show how the Integrated Risk-based Safety Index works for process units. Based on the information of fixed bed process for hydrogen dioxide provided by SINOPEC, several basic units were selected for analysis. Fixed bed process for hydrogen dioxide consists of four main units: hydrogenation, oxidation unit, extraction unit, and process unit (Fig. 5).

Table 6

Selected equipment at stage 2

S.no.	Equipment type	Equipment sub-type
1	Pump	
1.1		Centrifugal
1.2		Reciprocating
2	Compressor	
2.1		Centrifugal
2.2		Reciprocating
3	Heat exchanger	
3.1		Shell and tube
3.2		Air cooled
3.3		Plate type
4	Pipes	
5	Tanks	
6	Pressure vessels	
7	Reactors	
8	Boilers	

Table 7

Dependency of failure rate for various equipments

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

In the case study, we assumed 3 leakage scenarios for each column and calculated the risk. According to the limited process information, physical explosion index as well as dust explosion index was not adopted for the current case. Moreover, since this process had hydrogen dioxide involved in the whole process, reaction runaway scenario was also considered for extraction column as an example. Thus, 4 scenarios were analyzed for stage 1: hydrogenation column leakage scenario, oxidation column leakage scenario, extraction column leakage scenario, and extraction column exothermic runaway scenario. For leakage scenario, 10 min will be used as the time duration for risk analysis. Moreover, worst case scenario was adopted, namely maximum operating temperature and pressure were used for calculation, and so did the leakage size relevant to piping size. Among four piping diameters (50 mm, 80 mm, 200 mm and 350 mm), 350 mm was chosen as the case for leakage hole size.

According to the process, chemicals involved in each unit are roughly listed as below. The flow rate was assumed to be consistent in all the units, and the intermediate chemicals that produced during the process were not considered. For hydrogenation unit, chemicals involved are triethyl phosphate, trimethylbenzene (various isomers), methylcyclohexyl acetate, 2-ethylanthraquinone, and hydrogen. For oxidation unit, chemicals involved are triethyl phosphate, trimethylbenzene (various isomers), methylcyclohexyl acetate, 2-ethylanthraquinone, and hydrogen dioxide. For extraction unit, chemicals involved are triethyl phosphate, trimethylbenzene (various isomers), methylcyclohexyl acetate, 2-ethylanthraquinone, and hydrogen dioxide.

Take the hydrogenation column leakage scenario for example. For the hydrogenation unit, input data needed is shown in Table 9.

For Equipment Risk Index (ERI) calculation, the equipment type is reactor. Since the leak hole size of 350 mm is within the range of 50–500 mm, the hole size of 500 mm was chosen to get the data of failure rate for reactor from database. It is 0.00005 Failure Rate (/year). The result for ERI is 0.006895 for flammability and 0.05011 for explosivity.

According to current information, the hydrogenation column has several control barriers as follows: high temperature/pressure alarm, high temperature/pressure interlocking, high pressure interlocking of hydrogen, and safety valve. For case study, barriers selected are operational interlock loop — electronic DCS or single loop. Then, the result for control barrier operational interlock loop — electronic DCS or single loop is 0.0006895 for flammability and 0.005011 for explosivity. To conclude, this hydrogenation column leakage scenario has a risk index as follows (Tables 10 and 11).

Table 8

List of safety controls and PFD values [18,19]

No.	Safeguard/control	Classification type		Type of control		Affected sub-index					PFD	PFD mean value	Reference (for PFD value)
		Active	Passive	Preventive	Mitigative	Fire	Explosion	Toxic	Dust E	Physical E			
1	Pressure relief valve		x	x		x	x	x		x	$(1 \times 10^{-1})-(1 \times 10^{-5})$	1.00×10^{-2}	CCPS LOPA
2	Dike (auditable)		x		x	x	x	x			$(1 \times 10^{-2})-(1 \times 10^{-3})$	1.00×10^{-2}	CCPS LOPA
3	Blast wall		x		x		x				$(1 \times 10^{-2})-(1 \times 10^{-3})$	1.00×10^{-3}	CCPS LOPA
4	Fire proofing		x		x	x					$(1 \times 10^{-2})-(1 \times 10^{-3})$	1.00×10^{-2}	CCPS LOPA
5	Open vent		x	x		x	x	x	x		$(1 \times 10^{-2})-(1 \times 10^{-3})$	1.00×10^{-2}	CCPS LOPA
6	Flame/detonation Arrestor		x		x	x	x				$(1 \times 10^{-2})-(1 \times 10^{-3})$	1.00×10^{-2}	CCPS LOPA
7	Operational interlock loop - pneumatic	x		x		x	x	x			2.00×10^{-1}	2.00×10^{-1}	IEC 61511
8	Operational interlock loop - electronic DCS or single loop	x		x		x	x	x			1.00×10^{-1}	1.0×10^{-1}	IEC 61511
9	Check valves - for reverse flow only	x		x		x	x	x			$(0.03 \times 10^{-3})-(6.68 \times 10^{-3})$	0.00161	CCPS GPERD
10	Check valves - dual	x		x		x	x	x			$(0.285 \times 10^{-3})-(6.73 \times 10^{-3})$	0.0022	CCPS GPERD
11	Purge system	x		x		x	x	x			1×10^{-2}	1.00×10^{-2}	OREDA
12	Manual emergency depressuring valve	x		x		x	x	x			1×10^{-1}	1.00×10^{-1}	OREDA
13	Regulators - pressure	x		x		x	x	x			1.00×10^{-2}	1.00×10^{-2}	OREDA
14	Rupture disks - Independent	x		x		x	x	x		x	$(1 \times 10^{-1})-(1 \times 10^{-5})$	1.00×10^{-2}	CCPS LOPA
15	Vents (atmospheric vent on a tank vessel)		x	x		x	x	x			$(10^{-3})-(10^{-5})$ per year		CCPS LOPA
16	Fire wall		x		x	x					$(10^{-2})-(10^{-3})$		CCPS LOPA
17	Dike (non-auditable)		x		x	x	x				$(10^{-2})-(10^{-3})$		CCPS LOPA
18	Emergency response	x			x	x	x	x	x	x	(1×10^{-1})		Shell LOPA training database
19	Fire detection	x			x	x	x				$(0.019 \times 10^{-6})-(4.41 \times 10^{-6})/h$		CCPS GPERD
20	Firewater system	x			x	x	x		x	x	0.01		OGP - Appendix I
21	Deluge system	x			x	x	x	x	x	x	0.015		OGP - Appendix I
22	sprinkler system	x			x	x	x	x	x	x	0.005		OGP - Appendix I
23	SIF SIL 1	x		x		x	x	x			$(1 \times 10^{-1})-(1 \times 10^{-2})$		CCPS LOPA
24	SIF SIL 2	x		x		x	x	x			$(1 \times 10^{-2})-(1 \times 10^{-3})$		CCPS LOPA
25	SIF SIL 3	x		x		x	x	x			$(1 \times 10^{-3})-(1 \times 10^{-4})$		CCPS LOPA
26	Underground drainage system		x		x	x	x	x			$(1 \times 10^{-2})-(1 \times 10^{-3})$	1.00×10^{-2}	CCPS LOPA

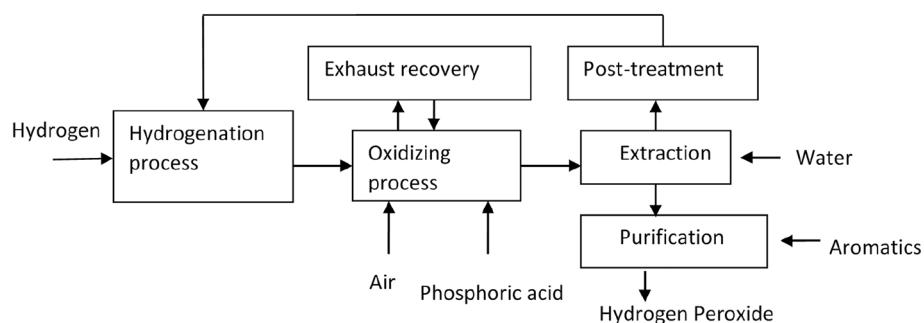
**Fig. 5.** Hydrogen dioxide process.

Table 9

Input data for hydrogenation unit

	Pressure/Pa	Temperature/°C	Leak hole/mm	Quantity/m ³
Hydrogen	401274.87	60	350	1173.16

Table 10

Risk index for hydrogenation column leakage scenario

	Distance/m	Stage 1 index	Stage 2 index	Stage 3 index
Flammability	9.3218	0.3585	0.006895	0.0006895
Explosivity	130.2635	2.6056	0.0501	0.005011

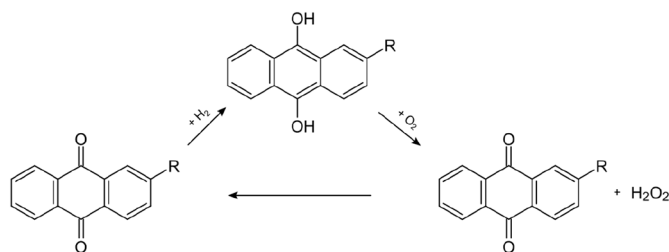
Table 11

Risk index for oxidation column leakage scenario

	Distance/m	Stage 1 index	Stage 2 index	Stage 3 index
Toxicity	19.8244	0.03961	0.0007617	0.00007617

Similarly, the leakage scenario for oxidation column and extraction column has a risk index as follows.

For runaway index, considering the process reaction (Fig. 6):

**Fig. 6.** Hydrogen dioxide reaction process.

The entire process may include hydrogenation, oxidation, as well as hydrogen dioxide thermal decomposition. For the extraction column, the decomposition reaction of hydrogen dioxide may take place. According to the information given, the input for this part is as follows (Tables 12 and 13).

Table 12

Input data for extraction column

	Pressure/Pa	Temperature/°C	Leak hole/mm	Quantity/m ³
Hydrogen dioxide	101352.932	50	350	1.5141

Table 13

Input data for runaway index (1cal = 4.1868 J)

	Reaction type	Heat release/cal·g ⁻¹	Adiabatic temperature rise/°C	(dT/dt) _{max} /°C·min ⁻¹
Extraction column	Decomposition	688.8145	24.2	712

Input values selected for the consideration of runaway index are as follows.

For the risk factor, since the process has hydrogen dioxide, and is sensitive to contaminants, it should be considered. For the safety factor, it has a reliable stirring system, a reliable cooling system, an automatic device to avoid incorrect mixing, updated information, a complete operating manual, an emergency power for control systems, and a fixed emergency cooling system. Above all, the stage 2 risk index and the stage 3 risk index of the runaway scenario of extraction column are 3.25 and 3.07, respectively.

4. Conclusions

This study developed a novel safety index to evaluate existing technologies for their safety levels and guide inherently safer design. The index system consisted of major hazards including fire, explosion, toxic release, dust explosion, physical explosion, and runaway. Moreover, the integrated life cycle approach considered chemical hazards, equipment failure rates and safety measures in this risk-based index. The integrated method using Neural Network and PHAST simulation was used to develop fire, chemical explosion and toxic indices. This safety index can be used to evaluate the risk level of petrochemical facilities by quantitatively 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 hydrogen dioxide synthesis was presented for the validation of the index system developed, which showed its capability for evaluating the safety level of process facilities. As the next step of the process to compare and select the inherently safer design, an interactive tool is necessary in order for the user to apply the 3 stages to different scenarios depending on the possible design specifications. The overall process of development of the tool, as well as the user experience with the tool, should be built basically in three main steps: 1) user parameter input, 2) background calculations, and 3) post-processing and reporting.

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